MML-Workshop 2021
November 22-24

Book of Abstracts

https://indico.gsi.de/e/MML_WK_2021

Contribution ID: **179** Type: **Invited Talk**

Introduction into the Program from Matter to Materials and Life

Monday, November 22, 2021 9:00 AM (20 minutes)

The research of the program aims to gain unique insights into the properties of matter and materials not accessible on a conventional laboratory scale. It addresses central questions related to an improved understanding and control of electronic and molecular processes at all relevant length and time scales, e.g. as a prerequisite for the development of novel functional materials and better-targeted drugs. Of central importance for this research is the focus and further development of our internationally outstanding user facilities for photons, neutrons, ions and highest electro-magnetic fields. In the presentation, a short overview of the current developments and challenges related to our research program and facilities will be given.

Primary author: STÖHLKER, Thomas (GSI & HI Jena)

Presenter: STÖHLKER, Thomas (GSI & HI Jena)

Session Classification: Session A

Contribution ID: **189** Type: **Invited Talk**

FISCOV

Monday, November 22, 2021 9:20 AM (20 minutes)

Presenter: WEISS, Manfred (Macromolecular Crystallography, Helmholtz-Zentrum Berlin)

Session Classification: Session A

Contribution ID: **143** Type: **Invited Talk**

Fragment screening against the SARS-CoV-2 macrodomain

Monday, November 22, 2021 9:40 AM (20 minutes)

The viral macrodomain Nsp3b is an important pathogenicity factor during infection with coronaviruses, including SARS CoV-2. Nsp3b inhibits the antiviral immune response in infected cells by binding and removing post-translational ADP-ribosylation through its ADP-ribosyl hydrolase activity. Studies in other coronaviruses have shown that mutations affecting this activity severely reduce viral pathogenicity, making Nsp3b is an attractive target for the development of antiviral drugs.

In prior studies we discovered a small molecule compound that binds to parts of the Nsp3b active site with low micromolar affinity. To further extend this initial hit and identify additional binders in other regions of the active site, we conducted X-ray crystallographic fragment screening, using selected fragments and the F2X-Entry fragment library developed at HZB. With this approach, we found 23 hits in the Nsp3b active site, including several fragments that show great potential to be developed into lead-like molecules against SARS CoV-2 Nsp3b.

Primary author: LENNARTZ, Frank (Macromolecular Crystallography, Helmholtz-Zentrum Berlin)

Co-authors: Dr WOLLENHAUPT, Jan (Macromolecular Crystallography, Helmholtz-Zentrum Berlin); LINHARD, Verena (Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt); Prof. SCHWALBE, Harald (Institute for Organic Chemistry and Chemical Biology, Goethe-University Frank-furt); Dr WEISS, Manfred (Macromolecular Crystallography, Helmholtz-Zentrum Berlin)

Presenter: LENNARTZ, Frank (Macromolecular Crystallography, Helmholtz-Zentrum Berlin)

Session Classi ication: Session A

Contribution ID: **126** Type: **Invited Talk**

Statistical crystallography reveals correlated motions of SARS-CoV-2 Mpro

Monday, November 22, 2021 10:00 AM (20 minutes)

The atomic motions of proteins make up life at the most fundamental scale. Imaging these motions remains a grand challenge, as such imaging would enable us to understand how proteins fold, how enzymes catalyze chemical reactions, and how signals are communicated via protein matter. Here, the study of an unprecedented number of protein crystals (>10 000), has enabled us to measure information transfer through a protein's structure. The crystals, obtained during a drug screening campaign at DESY against the main protease (Mpro) from SARS-CoV-2, show significant structural variability, even across drug-free datasets obtained under nominally identical conditions. These structural fluctuations from crystal-to-crystal reproduce dynamics we might expect in solution: they qualitatively reproduce long MD simulations. Further, they allow us to predict which parts of the protein are involved in allosterically regulating its function. Our results suggest that it is time to move beyond single crystals and pursue a *statistical* crystallography.

Primary author: LANE, Thomas (Deutsches Elektronen Synchrotron)

Presenter: LANE, Thomas (Deutsches Elektronen Synchrotron)

Session Classification: Session A

Contribution ID: **77** Type: **Invited Talk**

Milli-Watt average power ultrafast XUV sources and applications

Monday, November 22, 2021 10:20 AM (20 minutes)

High harmonic generation (HHG) enables laser-like extreme-ultraviolet (XUV) radiation with ultrashort pulse duration in a compact table-top setup. These sources already enabled a plethora of applications in fields as diverse as physics, chemistry, biology and material sciences. In this contribution the up-to-date most powerful HHG-based XUV source is presented. It delivers an average power of 13 mW at a photon energy of 26.5 eV, exceeding previous demonstrations by more than one order of magnitude. This is enabled by driving the HHG process with frequency doubled and post-compressed Yb-fiber laser, delivering a unique combination of sub-20 fs pulse duration, 515 nm wavelength and a high average power of 50 W.
Furthermore, first pioneering experiments enabled by this kind of HHG source are presented: XUV interferometry on the attosecond time scale and photo-ionization of C+ ions at the ion storage ring CRYRING.

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Presenter: KLAS, Robert (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classification: Session A

Contribution ID: **190** Type: **Invited Talk**

Large-scale facilities for quantum applications

Monday, November 22, 2021 11:00 AM (20 minutes)

Presenter: ASTAKHOV, Georgy V. (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Session B

Contribution ID: **133** Type: **Invited Talk**

Coherent control of collective nuclear quantum states via transient magnons

Monday, November 22, 2021 11:20 AM (20 minutes)

Dynamic control of quantum systems at X-ray energies is a major challenge in today's X-ray quantum optics. Many concepts known in the lower energy regime are not feasible due to the lack of appropriate X-ray laser sources. Thus, new schemes for dynamic control are called for. We measure and coherently control the phase of a collective quantum system that is embedded in a solid-state host by excitation of a solid's quasi particle. The quantum phase of a collectively excited nuclear state is controlled via transient magnons with a precision of 1 zeptosecond and a timing stability below 50 ys. The experiment demonstrates zeptosecond interferometry and shows that transient quasi-particles enable accurate control of quantum systems embedded in condensed matter environments. The technique opens new ways to precision quantum metrology.

Primary author: BOCKLAGE, Lars (DESY)

Presenter: BOCKLAGE, Lars (DESY)

Session Classification: Session B

Contribution ID: **31** Type: **Invited Talk**

Micro structures cut from crystalline quantum materials for research under challenging conditions

Monday, November 22, 2021 11:40 AM (20 minutes)

In order to study novel quantum materials, experiments are pushed to their limits in terms of setup dimensions and resolution. Major challenges for experiments with crystalline materials are limited sizes and varying shapes. Micromachining assisted by a focused ion beam (FIB) with nanometer precision can be a powerful approach for the creation of crystalline mesoscale devices with typical sizes of 10 nm to 100 μm. This range covers many of the relevant length scales in quantum materials. At the Dresden High Magnetic Field Laboratory, we are able to test these devices under challenging conditions, such as pulsed magnetic fields of close to 100 T, temperatures down to 10 mK, or pressures of up to 100 kbar.
In this talk, I will exemplify some of our recent projects that benefited from FIB assisted micropatterning, covering heavy-fermion metals, unconventional superconductivity and magnetism, and topological magnetic textures.

Primary author: HELM, Toni (Helmholtz-Zentrum Dresden-Rossendorf)

Presenter: HELM, Toni (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Session B

Contribution ID: **123** Type: **Invited Talk**

Exploring ultrafast terahertz-driven processes at the TELBE facility

Monday, November 22, 2021 12:00 PM (20 minutes)

Strong-field terahertz (THz) radiation offers a direct way to resonantly drive highly relevant low-energy modes in matter, e.g., lattice vibrations, molecular rotations, spin precession and the motion of (quasi-)free electrons. Using these pulses as a pump in ultrafast experiments enables the study of dynamic processes in solid-state, chemical and eventually biological systems. The TELBE THz facility at HZDR is a strong-field THz-source offering multicycle, CEP stable THz pulses with an exceptionally high spectral density at a repetition rate up to 500 kHz. Therefore, TELBE is ideally suited for the research on THz-driven nonlinear processes, from THz high harmonic generation to Higgs-Spectroscopy in superconductors. In this contribution, we present recent accomplishments at TELBE and discuss key directions for PoF IV.

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Presenter: DEINERT, Jan-Christoph (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Session B

Contribution ID: **45** Type: **Invited Talk**

Gold-implanted germanium as a material for ultrabroadband THz applications

Monday, November 22, 2021 12:20 PM (20 minutes)

Photoconductive materials are widely used for generation, detection or modulation of terahertz radiation. However, the bandwidth of photoconductive devices is often limited by the opacity bands related to polar optical phonons. Germanium as a non-polar semiconductor is free from this drawback and its operation spectrum is virtually gapless. However, the utilization of Ge for photoconductive terahertz devices was limited by relatively long carrier lifetimes making it incompatible with typical laser oscillators.

We show that a gold implantation can reduce the carrier lifetime in Ge down to sub-nanosecond level. Using this modified material, we demonstrate an ultrabroadband photoconductive THz emitter with a gapless spectrum up to 70 THz. In addition, we use the same gold-doped Ge as pulse-picker for terahertz pulses from FELBE free-electron laser in a broad range of infrared wavelengths. The demonstrated device can be used for the cavity dumping to achieve higher pulse energy and lower average power.

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Presenter: PASHKIN, Alexej (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Session B

Contribution ID: **1** Type: **Poster**

Nozzle design for FLASH irradiation of single mice eyes

Monday, November 22, 2021 1:30 PM (1h 40m)

The Charité – Universitätsmedizin Berlin is treating about 220 to 270 patients per year with intra ocular tumors like uveal melanoma at the proton facility of the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB). In order to get a better understanding of the side effects, e.g. radiation retinopathy, animal studies are performed in parallel: a single eye of a mouse is irradiated with a small field of 9 mm diameter and a penetration depth of 5 mm. The second – non irradiated – eye is used as an internal control.
FLASH irradiations with dose rates of 40 Gy/s or more seem to have a great potential to treat tumors as effective as conventional radiotherapy but with less side effects, as demonstrated by different animal studies. The idea is to repeat the mice irradiations under FLASH conditions.

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Presenter: DENKER, Andrea

Session Classification: Poster Session 1

Contribution ID: **3** Type: **Poster**

Investigating the cellular mechanism of coronavirus inhibition by anti-depressants

Monday, November 22, 2021 1:30 PM (1h 40m)

FDA-approved anti-depressant drugs have been shown to inhibit coronavirus replication in cell culture models and also to reduce hospitalization in high-risk patients, but their mechanism of action remains unknown. To investigate this, we are combining X-ray microscopy performed at the HZB U41 beamline with fluorescence and electron microscopy to track cat coronavirus uptake and processing in cat kidney cells, whose infection we find is also blocked by the anti-depressants. With no drugs, we detect virus on filopodia and in late endosomes. With an anti-depressant, we detect significant alterations in filopodial and late-endosome morphology, suggesting that the drugs may act at both of these sites. Our work towards a better understanding of the inhibitory mechanism(s) of the anti-depressants will not only aid the efforts to treat the ongoing pandemic of SARS CoV-2, but also the development of treatments for any future pandemics caused by coronaviruses.

Primary authors: MCNALLY, James (Helmholtz Zentrum Berlin); Dr NIE, Chuanxiong (Free University Berlin); Mr DYHR, Michael (Free University Berlin, Helmholtz Zentrum Berlin)

Presenter: MCNALLY, James (Helmholtz Zentrum Berlin)

Session Classification: Poster Session 1

Contribution ID: **8** Type: **Poster**

Real-time insight during the rapid formation of ultra-thin gold layers on polymers

Monday, November 22, 2021 1:30 PM (1h 40m)

Hybrid nanomaterials composed of polymers covered with ultra-thin metal layers are widely used in advanced technologies – such as OLEDs, OPVs, sensors, or fuel cells. Ultra-thin metal layers are created by sputter deposition in few seconds in industrial applications. Using sub-millisecond GISAXS at the P03 beamline of PETRA III allowed us to examine the growth of an ultra-thin gold layer on polymeric substrate with a sub-nanometer spatial resolution. In the first few milliseconds, a fraction of the incoming gold atoms manages to penetrate the polymer matrix, while others begin to form vertical diatomic clusters. Subsurface enrichment and doping of polymer layers with gold atoms changes the material's thermodynamic behavior, which could be exploited in some applications. This real-time observation of nanolayer formation could be used to study the effect of different deposition conditions, e.g., substrate temperatures, and allow us to control and optimize the manufacturing of metal-polymer hybrid materials.

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Co-authors: Dr STRUNSKUS, Thomas (CAU); Dr KÖRSTGENS, Volker (TUM); Prof. MÜLLER-BUSCHBAUM, Peter (TUM); Prof. FAUPEL, Franz (CAU); Prof. ROTH, Stephan V. (DESY KTH)

Presenter: SCHWARTZKOPF, Matthias (DESY)

Session Classification: Poster Session 1

Contribution ID: **9** Type: **Poster**

3d charge distributions beyond the oxidation state revealed by high resolution x-ray absorption spectroscopy

Monday, November 22, 2021 1:30 PM (1h 40m)

Connecting physical charge distributions and formally derived oxidation states in transition metal complexes is of high interest to modern chemistry and material science. With this study we provide a systematic investigation of changes in the iron L-edge excitation energy depending on the charge distribution on the iron center of gas phase diatomic FeX+ (X = F, Cl, Br, I) using high resolution x-ray absorption spectroscopy. A comparison of the iron halide samples with Fe+ revealed a shift in excitation energy towards lower energies with respect to the Fe+ and along the FeX+ series. The experimentally determined excitation energy shifts correlate with the electronegativity of the halogen and are attributed to an increase in 3d derived orbital population supported by charge transfer multiplet calculations. Hence, we show a general dependence of transition metal 3d derived orbital population connecting two oxidation states that by definition corresponds to integer occupation of atomic orbitals.

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Presenter: Mr FLACH, Max (Helmholtz-Zemtrum Berlin für Material und Energie)

Session Classification: Poster Session 1

Contribution ID: **10** Type: **Poster**

Surface treatment procedures to mitigate desorption processes induced by swift heavy ions

Monday, November 22, 2021 1:30 PM (1h 40m)

Ion-induced desorption is a serious limitation for stable operation of high beam intensities in heavy ion synchrotrons. To better understand and control the influence of material and surface factors desorption measurements with swift heavy ions (Ca and Au at 4.8 MeV/u) were conducted with focus on oxygen-free copper and tungsten samples. The surfaces were treated by different combinations of milling, lapping, polishing, etching and sputtering. Some of the samples were coated by carbon, titanium nitride or TiZrV. For all tested samples desorption yields for H2, H2O, CO, CO2, O2 and Ar will be presented. For copper, surface cleaning by sputtering with 5 keV argon ions reduces the desorption yield significantly. Another promising method to reduce ion-induced desorption is thermal annealing at 400 ℃ for about 4 h under ultra-high vacuum conditions.

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Presenter: VELTHAUS, Verena (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classi ication: Poster Session 1

Contribution ID: **13** Type: **Poster**

Telecom single-photon emitters in silicon for scalable quantum photonics

Monday, November 22, 2021 1:30 PM (1h 40m)

Single-photon sources emitting indistinguishable photons on demand in the optical telecom O and C bands are key building blocks for long-haul fiber-optic quantum communication and quantum photonic integrated circuits. Silicon with its stable oxide (SiO2) and its mature computer-chip manufacturing process would provide a crucial advantage in building large-scale quantum networks, enabling a link between quantum computing and quantum communication in the same framework.
This work reports the creation of single-photon emitters with a high brightness approaching 105 counts per second in commercial silicon-on-insulator (SOI) wafers. The emission occurs in the infrared spectral range with a spectrally narrow zero-phonon line in the telecom O-band and shows a high photostability even after days of continuous operation. The origin of the emitters is attributed to one of the carbon-related color centers in silicon, the so-called G center, allowing purification with the 12C and 28Si isotopes.

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Presenter: Dr BERENCÉN, Yonder (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classi ication: Poster Session 1

Contribution ID: **14** Type: **Poster**

Field-induced magnetic order and exchange anisotropy of the triangular-latttice antiferromagnets NaYbCh2 (Ch = O, S, Se)

Monday, November 22, 2021 1:30 PM (1h 40m)

The Yb-based delafossites NaYbCh2 (Ch = O, S, Se) are triangular-lattice antiferromagnets with a trigonal crystal structure (space group □-3□). In these compounds, spin-orbit coupling and the crystal electric field lead to a pronounced magnetic anisotropy and a pseudospin-1/2 ground state at low temperatures. The chalcogen series provides the possibility for tuning the interlayer distance and the associated exchange couplings by changing the chemical composition. The absence of magnetic long-range order at zero field is suggestive for a quantum spin-liquid ground state. From specific-heat and magnetization experiments, magnetically ordered states were observed for applied fields exceeding 2 T for all three compounds. For in-plane fields of several tesla, a plateau-like feature indicates an up-up-down spin arrangement. Furthermore, measurements of the magnetization up to very high magnetic fields of 30 T allow to probe the saturation fields and polarized moments and, thus, the determination of the anisotropic exchange couplings.

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Presenter: LUTHER, Sven (Hochfeld-Magnetlabor (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Session Classi ication: Poster Session 1

Contribution ID: **15** Type: **Poster**

Transport Properties of Soft-Etched Polyimide Membranes

Monday, November 22, 2021 1:30 PM (1h 40m)

The soft-etch (SE) technique is used to Fabricate subnanopores in heavy ion tracked polyimide (PI) membrane. In SE methods ion tracks are selectively dissolved without affecting the bulk material by using an organic solvent. The ion transport properties of SE-PI membrane are studied in various electrolyte solutions containing metal cations, alkali metal-crown ether complexes and alkylammonium cations under symmetric and asymmetric electrolyte conditions. The experimental findings show that the SE-PI membranes have the ability to discriminate alkali cations from divalent metal cations. Moreover, the results suggest that only the [Li(12C4)]+ complex can translocate freely through the pores because significant current decreases are observed for the cases of the [Na(15C5)]+ and [K(18C6)]+ complexes. Based on the outstanding stability and ultrahigh discrimination capability, we envision that such SE-PI membrane can be successfully employed in a variety of filtration devices.

Primary authors: ALI, Mubarak (Technische Universität(TUDA)); Dr NASIR, Saima (GSI/ TU darmstadt); Ms FROEHLICH, Kristina (TU Darmstadt); Prof. ENSINGER, Wolfgang

Presenter: ALI, Mubarak (Technische Universität(TUDA))

Session Classification: Poster Session 1

Contribution ID: **16** Type: **Poster**

Morphology and growth behavior of Cu nanoparticles on the vicinal ZnO(10-14) surface

Monday, November 22, 2021 1:30 PM (1h 40m)

We investigated Cu nanoparticles (NPs) grown under ultra high vacuum conditions on ZnO(10-14) single crystal surfaces by scanning tunneling microscopy, high energy grazing incidence x-ray diffraction and scanning electron microscopy. The NPs show alignment of the Cu [111] with the ZnO [0001] crystal direction, which is at an angle of 24.8° to the ZnO(10-14) substrate's surface normal. Due to this tilt, the NPs exhibit a shape with a large fraction of high indexed facets such as (335), (221), (113) and (55-1). In addition, the direct interaction of subsequent Cu(111) planes to the underlying substrate results in unequal amounts of ABCA and ACBA stacked NPs. Small NPs are found to interact strongly with the vicinal surface, giving rise to a surface corrugation with a multiple of the surface step distance. The high density of low-coordinated Cu surface atoms potentially increases the overall catalytic activity for methanol synthesis and CO2 hydrogenation reactions.

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Presenter: GLEIßNER, Robert (Center for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY)

Session Classification: Poster Session 1

Contribution ID: **17** Type: **Poster**

NMR investigations of the 2D Heisenberg system CuPOF under pressure

Monday, November 22, 2021 1:30 PM (1h 40m)

The molecular-based material $(Cu(pz)_2(2\text{-}OHpy)_2)(PF_6)_2$ (CuPOF) is an excellent realization of a two-dimensional square-lattice $S = 1/2$ Heisenberg antiferromagnet, with intralayer and interlayer exchange-coupling constants of $J/k_B = 6.8$ K and $J' \approx 10^{-4}J$, respectively. Previously reported NMR data revealed a low-temperature transition to commensurate antiferromagnetic (AFM) quasistatic long-range order (LRO), with a preceding crossover from Heisenberg to anisotropic XY behaviour. We present further NMR studies of the low-temperature correlations in magnetic fields up to 7T and temperatures down to 0.3K. The application of hydrostatic pressure up to 10kbar changes the interlayer coupling and, therefore, the magnetic correlations in the critical regime. The transition regime is probed by ^{1}H and ^{31}P spectroscopy and relaxometry, revealing a monotonic change of T_N with increasing pressure. The AFM LRO below T_N persists at high pressures, as revealed by a splitting of the ^{1}H NMR lines, stemming from the broken symmetry of the local spin polarization in the LRO regime.

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Presenter: BÄRTL, Florian (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Poster Session 1

Contribution ID: **20** Type: **Poster**

The precession dynamo experiment at HZDR

Monday, November 22, 2021 1:30 PM (1h 40m)

Cosmic magnetic fields exist on all scales, from planets and stars to galaxies and beyond. The generation of these fields via the hydromagnetic dynamo effect involves the formation of electrical currents by means of complex flows of conducting fluids or plasmas. At HZDR a related experiment is under construction within the project DRESDYN. In that experiment a precessing flow of liquid sodium will provide the required energy for magnetic field generation.

Here we address preliminary numerical and experimental studies aimed at the identification of parameter ranges where a dynamo can be expected. Our kinematic dynamo models show that dynamo action is possible just before the transition from a laminar flow state to vigorous turbulence where the flow structure is determined by a combination of axisymmetric and nonaxisymmetric large scale modes. By applying the derived scaling laws, the results can be directly applied to the parameters of the planned large device.

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Presenter: GIESECKE, Andre (HZDR)

Session Classification: Poster Session 1

Contribution ID: **21** Type: **Poster**

AXSIS S-band compact RF gun using pin cathode for photoemission

Monday, November 22, 2021 1:30 PM (1h 40m)

AXSIS RF gun is an S-band compact RF gun with a frequency of 2.998 GHz, which can accelerate the electrons up to 150 keV. The maximum power of a compact amplifier is 10 kW, so a pin-cathode has been used in the cavity in order to increase the RF electric field on the cathode up to 100 MV/m. A solenoid is also used just after the gun to focus the electron beam in the transverse direction. After the construction of this device, vacuum tests and RF tests show that there is good compatibility with the designs and simulations. By continuing the conditioning at high power and high current of the solenoid, the electron multipacting (created due to the entrapment of the electrons) gradually disappears and we can start the photoemission on the pin cathode.

Primary author: Mr BAZRAFSHAN, Reza

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Presenter: Mr BAZRAFSHAN, Reza

Session Classification: Poster Session 1

Contribution ID: **22** Type: **Poster**

Status of Cyogenic Current Comperators (CCCs) for beamlines

Monday, November 22, 2021 1:30 PM (1h 40m)

CCCs are highly sensitive current meters that, using superconducting effects, are able to measure charged particle streams in the nA range non-destructively and absolutely. Two CCC systems are in use in beamlines and further CCC-sensors are in laboratory operation. After 2 years of shutdown, the CERN-Nb-CCC at CERN-AD was put back into operation, currently measured beam currents were 3.3 µA. The GSI-Nb-CCC-XD was tested with its newly developed beam cryostat in the CRYRING. Low Ne3+ beam currents in the range of 150nA with a resolution of 10nA and high U91+ beam currents in the range 20µA with a noise level of approx. 1µA were measured. The further development of cost-effective Pb-CCC with and without cores was driven forward in in the CDL Jena (FSU-Jena, Leibniz-IPHT and HI-Jena). Key results from the completed BMBF project 18-21 are presented here and the goals for the new funding period are outlined.

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Session Classification: Poster Session 1

Contribution ID: **26** Type: **Poster**

Enabling extended collaborative research in crystallography with Amarcord.

Monday, November 22, 2021 1:30 PM (1h 40m)

Amarcord was started as an attempt to ease the collaboration between researchers in crystallography screening experiments related to COVID-19. This database has proven to be an invaluable tool in such a large collaboration. For researchers, it meant (1) speed and (2) better results, because many experts from different fields were all able to contribute to the same task, without duplicating one another's work. In the end, it means more drug leads found with less effort in less time. The database in its current status provides a web-interface summarizing the samples and measurement conditions. Data analysis results can be manually added at posteriori, and we are working on extending it as a framework for analysis workflows. Such a tool enables a new type of multidimensional experiments (large parameter spaces of structures vs time, ligand, temperature, pH…). The generated metadata can be used to drive discoveries and insights.

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Presenter: CARNIS, Jerome (DESY)

Session Classification: Poster Session 1

Contribution ID: **27** Type: **Poster**

High current accelerator systems for future HBS: HBS Innovationpool Project

Monday, November 22, 2021 1:30 PM (1h 40m)

Compact accelerator-based neutron sources offer a promising route towards the next generation of neutron research facilities. They do not require research reactors or high-energy spallation sources as they efficiently utilize nuclear processes at low acceleration energies. For the research and development of the various components and areas relevant to establish a high brilliance accelerator based neutron source an Innovation Pool project on "High current accelerator systems for future HBS" has been set up within the Research Field Matter of the Helmholtz Association staring in 2019. Research and development in this project deal with i) linear pulsed proton accelerator cavities, (GSI HI Mainz), ii) fast proton beam multiplexing and beam dynamics (FZJ), iii) neutron target- and moderator development (FZJ), iv) neutron beam extraction and instrumentation (HZG) and neutron imaging and irradiation experiments (HZDR). Results of this work till now will be reviewed.

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Session Classi ication: Poster Session 1

Contribution ID: **28** Type: **Poster**

Disproportionation in gas-phase di-manganese oxide cluster revealed by X-ray absorption spectroscopy

Monday, November 22, 2021 1:30 PM (1h 40m)

Photosystem II, with its active center a $CaMn_4O_5$ cluster (OEC), is essential for photosynthesis and therefore O_2 production in nature [1]. The understanding of the electronic structure and properties of this complex plays important role in designing artificial water-oxidizing complexes. During oxygen formation the OEC undergoes five distinct states called S_{0-4} forming the Kok cycle. Despite detailed knowledge of S_0 through S_3 there is still a lack of information on S4 due to challenges of preparing OEC in S_4 [2]. However, two major competing models for S_4 have been proposed in the literature which involve distinctively different oxidation states namely Mn(IV) (and an oxygen radical) and Mn(V), respectively.
Here, we report on di-manganese oxide cluster $Mn_2O_3^+$ which forms a subunit of the OEC. Using X-ray absorption spectroscopy we find an unusual charge disproportionation in $Mn_2O_3^+$, where manganese atoms in oxidation states $+2$ and $+5$, respectively.

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Session Classification: Poster Session 1

Contribution ID: **29** Type: **Poster**

Characterizing the Ionization Potential Depression in Dense Plasmas with High-Precision Spectrally Resolved X-ray Scattering

Monday, November 22, 2021 1:30 PM (1h 40m)

Details of a recent experiment at the European XFEL will be presented, studying the ultrafast creation of dense plasmas by isochoric heating, and characterizing their properties. The high-precision X-ray scattering diagnostic used is particularly well-suited to probe the ionization potential depression as well as ionization and temperature. This approach has a high potential to resolve existing discrepancies on ionization potential depression models that are important for modelling celestial bodies like giant planets, Brown Dwarfs and stars as well as for several technological applications including intense laser matter interaction and radiation damage research.

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Session Classification: Poster Session 1

Contribution ID: **30** Type: **Poster**

Dislocation Dynamics in Semiconductor Wafers Studied by 3D X-ray Diffraction Imaging

Monday, November 22, 2021 1:30 PM (1h 40m)

With the ongoing miniaturization of silicon (Si) based microelectronics, the understanding, prediction, and avoidance of processing-induced crystal defects like dislocations and their evolution become more and more relevant, thus motivating both scientific and industrial interest in their systematic investigation.
X-ray diffraction laminography (XDL) has recently been developed at KIT, enabling non-destructive 3D imaging of crystal defects with μm spatial resolution, in particular also in laterally extended samples like semiconductor wafers. The recent instrumental and related methodical progress, including well-defined and monitored thermal treatment of samples, now enables quasi *in situ* 3D investigations of dislocation dynamics in semiconductor wafers in industrially relevant conditions. We here present a quasi *in situ* study of the 3D evolution of individual dislocations in industrial Si wafers generated by fabrication-relevant heating conditions, their interaction within complex networks, as well as the relation of the observed dynamics with the driving thermal forces.

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Session Classification: Poster Session 1

Contribution ID: **32** Type: **Poster**

A 3D Risk Model to Assess Radiation-Induced Cardiotoxicity

Monday, November 22, 2021 1:30 PM (1h 40m)

The risk of developing cardiovascular disease after exposure to radiation increases with the received dose. However, underlying mechanisms are poorly understood.
We used cardiomyocytes generated from human embryonic stem cells in an organotypic 3D model, mirroring key features of the myocardium. After an in-depth characterization of the model, these clusters were irradiated with X-rays up to 2 Gy. Functional parameters of the contraction were measured and linked to changes in the proteome up to one month after the irradiation.
The video analysis of irradiated clusters revealed subtle changes in beat frequencies and decreases in rhythmicity compared to controls. Proteome changes point towards structural remodeling and a loss of contractile fibers as a result of the X-ray exposure.
Here, we propose an in vitro model suitable to screen radiation-induced cellular effects by testing beyond classical cardiotoxicity assays.

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Session Classification: Poster Session 1

Contribution ID: **33** Type: **Poster**

Bragg Magnifier Optics for Dose-Efficient X-Ray Imaging with µm-Resolution

Monday, November 22, 2021 1:30 PM (1h 40m)

High-resolution synchrotron X-ray imaging of biological samples, especially *in-vivo*, is often hindered by radiation damage. Many efforts have been made to reduce the dose, e.g., by phase-contrast-imaging. However, the detection efficiency of indirect converting, scintillator-based detector systems drops significantly with increasing energy and decreasing pixel size.

In order to overcome these limitations, we developed a novel Bragg Magnifier imaging setup based on asymmetrically cut Si-crystals (optimized for 28-31 keV). The system allows magnifying the sample image by a factor of up to 200 onto a large-area, highly efficient single-photon-counting detector. The system has a theoretical detection efficiency of 91% for a spatial resolution of about 1 µm – in contrast, an indirect detector achieves ~10% under comparable conditions.

Here, we present our novel instrumentation and first experimental results obtained at KIT synchrotron and PETRA III, demonstrating its potential for dose-efficient phase-contrast X-ray imaging of biological organisms and other radiation-sensitive samples.

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Session Classification: Poster Session 1

Contribution ID: **34** Type: **Poster**

Single alloy nanoparticle x-ray imaging during a catalytic reaction

Monday, November 22, 2021 1:30 PM (1h 40m)

The imaging of active nanoparticles represents a milestone in decoding heterogeneous catalysts' dynamics. We report the facet-resolved, surface strain state of a single PtRh alloy nanoparticle on SrTiO3 determined by coherent x-ray diffraction imaging under catalytic reaction conditions. Density functional theory calculations allow us to correlate the facet surface strain state to its reaction environment–dependent chemical composition. We find that the initially Pt-terminated nanoparticle surface gets Rh-enriched under CO oxidation reaction conditions. The local composition is facet orientation dependent, and the Rh enrichment is nonreversible under subsequent CO reduction. Tracking facet-resolved strain and composition under operando conditions is crucial for a rational design of more efficient heterogeneous catalysts with tailored activity, selectivity, and lifetime.

DOI: 10.1126/sciadv.abh0757

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Session Classification: Poster Session 1

Contribution ID: **36** Type: **Poster**

Molecular dynamics study of non-equilibrium dense plasmas with ionization potential depression

Monday, November 22, 2021 1:30 PM (1h 40m)

The advent of x-ray free-electron laser (XFEL), enables us to creat dense plasmas under non-local thermal equilibrium (NLTE) where the plasma screening effect appears mainly as ionization potential depression (IPD) or continuum lowering.

In this study, we employ XMDYN, a Monte-Carlo (MC) and molecular dynamic (MD) -based computational tool to simulate the dense materials interacting with intense XFEL pulses. To include the IPD for NLTE plasma environment, we propose a numerical method based on atomic energy shift due to the micro-field from MD simulations.
We validate the method and illustrate the merit of it by simulating an existing FEL-aluminum solid interaction experiment as a bench mark. The IPD effect are shown by turning it on and off and comparing the outcome such as charge state distribution, plasma temperature and so on. The IPD values are compared with Stewart-Pyatt (S-P) or Eker-Kröll (E-K) models and average-atom models for LTE systems.

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Session Classification: Poster Session 1

Contribution ID: **37** Type: **Poster**

Material-specific table-top EUV imaging

Monday, November 22, 2021 1:30 PM (1h 40m)

State-of-the art high harmonic sources nowadays provide coherent radiation in the extreme ultraviolet with high photon flux. This enables coherent imaging experiments that were so far only possible at large-scale research facilities (e.g. synchrotrons) on a laboratory scale. Here, we will present a new EUV microscope operating at a wavelength of 13.5 nm. It achieves a resolution of sub 20 nm and allows material-specific imaging of an integrated circuit.

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Session Classi ication: Poster Session 1

Contribution ID: **38** Type: **Poster**

Resonance-enhanced multiphoton ionization in the x-ray regime

Monday, November 22, 2021 1:30 PM (1h 40m)

Multiphoton ionization is one of the fundamental nonlinear processes when matter interacts with intense laser fields. In particular, REMPI has been a widely-used spectroscopic technique due to high sensitivity and selectivity. Extending REMPI to the x-ray regime, however, requires entirely different physical processes and interpretation, due to accompanying ultrafast Auger decay processes. We present a first observation of REMPI in the short wavelength regime using ultraintense x rays from the European XFEL. We observe nonlinear ionization to create Ar^{17+}, where photon energies are insufficient to directly ionize a $1s$ electron. With the aid of state-of-the-art theoretical modeling, we attribute the ionization to a two-color REMPI-like process where the second harmonic creates a $1s \rightarrow 2p$ transition and the fundamental pulse subsequently ionizes the system. This resonant phenomenon occurs not only for Ar^{16+}, but through multiple lower charge states, where multiple ionization competes with decay lifetimes, making x-ray REMPI distinctive from conventional REMPI.

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Session Classi ication: Poster Session 1

Contribution ID: **39** Type: **Poster**

Hierarchical in situ laminography applied for the study of damage formation in alloy sheets

Monday, November 22, 2021 1:30 PM (1h 40m)

Hierarchical *in situ* X-ray computed laminography (CL), developed at KIT, offers unique possibilities to investigate laterally extended samples on multiple scales. By means of KB-mirrors, the approach implements X-ray microscopy modalities. Fast online phase- and 3D reconstruction enables crucial hierarchical guidance during the *in situ* observation of the sample deformation, continuously allowing us to identify, zoom-in on and track local regions-of-interest inside the material.
Recently the method was employed to get a comprehensive view of damage formation in alloy sheets under engineering-relevant conditions, as typical e.g. for transport applications. The multiscale data obtained enables us to correlate mesoscopic information (e.g. strain bands) and nanoscale damage processes (e.g. void nucleation or coalescence).
Here we present the methodological development of KB-Mirror based hierarchical *in situ* laminography at meso- to nanoscale resolution and first exemplary results of the observation of damage formation in alloy sheets on multiple scales.

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Session Classification: Poster Session 1

Contribution ID: **41** Type: **Poster**

Ultrafast molecular dynamics induced by few-femtosecond ultraviolet excitation

Monday, November 22, 2021 1:30 PM (1h 40m)

Ultraviolet (UV) induced ultrafast processes in molecules are fundamental for their chemical and biological implications, however the investigation of few-fs electron dynamics has been barely explored, mostly due to the technological challenge of producing few-fs pulses in this spectral region.

Here, we present the first benchmark pump-probe experiments employing few-fs UV pulses combined with a 5-fs VIS/NIR probe. Electron Velocity Map Imaging (VMI) images and Time-of-Flight Mass Spectra (TOFMS) are simultaneously recorded as a function of the delay between the two pulses using a double-sided spectrometer.

In acetone, the kinetic energy of the emitted electrons the decay appears modulated by a 25 fs oscillation which starts immediately after the excitation. In iodomethane, instead, the few-fs temporal resolution of the experiment allows us to resolve the appearance of the iodine ion yield after 25 fs from the time overlap. The interpretation of the above-mentioned results is still preliminary.

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Session Classification: Poster Session 1

Contribution ID: **42** Type: **Poster**

FLASH THz beamline after FLASH2020+

Monday, November 22, 2021 1:30 PM (1h 40m)

The FLASH1 THz beamline at DESY provides intense THz pulses simultaneously to the FEL soft X-ray radiation for THz-XUV pump-probe experiments. After FLASH 2020+ project, a new semi-permanent endstation for the pump-probe experiments will be implemented and aims at various scientific researches such as solid state- and surface physics, surface chemistry, and especially femtomagnetism by various experimental geometries such as reflection- (for transverse magneto-optic Kerr effect, T-MOKE) or transmission (for magnetic small-angle X-ray scattering, SAXS) geometry under the operation mode called THz doubler. Online photon diagnostics for the THz pulses are under development and will provide the THz temporal- and spectral profile at the sample position on a single-shot basis employing electro-optic sampling (EOS).

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Presenters: GANG, Seung-gi (DESY); Dr PAN, Rui (DESY)

Session Classification: Poster Session 1

Contribution ID: **43** Type: **Poster**

Effect of doping technique on the structure and thermoelectric properties of P3HT-based thin films

Monday, November 22, 2021 1:30 PM (1h 40m)

Poly(3-hexylthiophen-2,5-diyl) (P3HT) is one of the most prominent semiconducting, conjugated polymers in the fields of organic electronics and photovoltaics. Besides its high electric conductivity, it shows thermoelectric properties when doped with metal chlorides or nanoparticles, i.e. gold (Au). This study aims for correlating process and fabrication parameters and the structural changes with the overall thermoelectric performance of P3HT and P3HT:PMMA films. We choose sprayed thin films, since they offer an excellent scalability in future industrial applica-tions and focus on two routes of gold (Au) doping, namely sputter and spray deposition techniques. The structure of the resulting polymer composites indicated distinct differences whether the gold is sprayed or grown on the surface as shown by ellipsometric, AFM, GISAXS/GI-WAXS as well as neutron and X-ray reflectivity measurements. This information will be crucial for improving the thermoelectric properties of thin films and providing a scalable approach for future industrial manufacturing.

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Session Classi ication: Poster Session 1

Contribution ID: **44** Type: **Poster**

Using XFELs to Probe Extreme Magnetic Fields in Relativistic High Power Laser Matter Interactions

Monday, November 22, 2021 1:30 PM (1h 40m)

The relativistic laser matter interaction is a complex interplay of ionization, extreme current densities, rapidly evolving strong fields and acceleration processes. Understanding the interaction physics is a challenging but highly rewarding endeavor. The recently commissioned X-Ray free electron lasers (XFELs) with unprecedented brightness and polarization purity open a new window for discovering the interior of solid-density plasmas created by relativistic laser interactions with matter, resolving the relevant femtosecond and nanometer scales experimentally. Here, we focus on discussing the feasibility of probing the Kilotesla to Megatesla-level magnetic fields by X-Ray polarimetry via Faraday rotation using XFELs. The synthetic simulations show that XFELs are capable to detect the extreme magnetic fields from relativistic laser interactions with solid and near-critical density targets[1,2].
[1] L. G. Huang, H. P. Schlenvoigt, H. Takabe, and T. E. Cowan, PoP24, 103115 (2017).
[2] T. Wang, T. Toncian, M. S. Wei, and A. V. Arefiev, PoP26, 013105 (2019).

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Session Classification: Poster Session 1

Contribution ID: **46** Type: **Poster**

Geo- and astrophysical motivations for the DRESDYN dynamo experiment

Monday, November 22, 2021 1:30 PM (1h 40m)

The DRESDYN precession dynamo experiment at HZDR is motivated by recent observational indications that planetary and stellar dynamos are susceptible to external forces. An unambiguous case in point is the appearance of the various Milankovitch cycles of the Earth's movement in the statistics of the geomagnetic field. A more controversially discussed example is the apparent synchronization of the Schwabe cycle of the solar dynamo with the 11.07-year spring-tide periodicity of the tidally dominant Venus-Earth-Jupiter system. We discuss some physical mechanisms which might be capable to synchronize the solar dynamo by those weak tidal forces. This dynamo model is then extended to respond also to the 19.86-year periodic motion of the Sun around the barycenter of the solar system. The emergent 193-year beat period is shown to be a candidate for the Suess-de Vries cycle. Finally, the possibility of chaotic transitions into grand-minima states is discussed.

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Presenter: STEFANI, Frank (HZDR)

Session Classification: Poster Session 1

Contribution ID: **47** Type: **Poster**

Status and Prospects of 3D Laminographic Imaging at KIT

Monday, November 22, 2021 1:30 PM (1h 40m)

At KIT, we are continuously progressing in the methodical and instrumental development of X-ray computed laminography (CL), which enables non-destructive hierarchical 3D characterization of flat and laterally extended objects. Combining screening large areas with zooming in on selected regions of interest with high 3D resolution, CL is particularly well suited for many *in situ* and *operando* studies under real-world conditions. Our pool of complementary instrumentation was established in collaboration with the ESRF and DESY and allows exploiting the unique X-ray beam properties of beamlines at KIT, ESRF, PETRA III/IV, and in the lab, thus covering different contrast modes and a wide range of length scales.
We will overview our new instrumental developments optimized for 4D *in situ* studies, the future prospects of our laminography portfolio, and our current application of CL to the 3D *in situ* characterization of metal sheets during tensile testing, which is crucial e.g. for transportation applications.

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Session Classification: Poster Session 1

Contribution ID: **48** Type: **Poster**

Real-time observation of a correlation-driven sub-3-fs charge migration in ionised adenine

Monday, November 22, 2021 1:30 PM (1h 40m)

For organisms to cope with ultraviolet sunlight and ionizing radiation which can damage critical molecule such as DNA, ultrafast relaxation processes offer a first line of defence (photostability). The complexity of such molecules makes it challenging to understand under which conditions ionization leads to bond-breakage. In our combined experimental and theoretical investigation, we find and time-resolve a correlation-driven electronic relaxation process with consequences for the molecular stability of the nucleobase adenine. After ionization by an isolated attosecond pulse in the extreme ultraviolet, the molecule usually dissociates but we were able to produce the intact adenine dication by waiting 2.3 fs for an electronic rearrangement to occur and then sending a near-infrared probe/control pulse. Theory identifies the underlying mechanism as shake-up to a particular orbital and shows an "inflation" effect where a significant portion of the electron density moves away from the plane of the molecule.

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Session Classification: Poster Session 1

Contribution ID: **49** Type: **Poster**

Towards multiscale simulations for matter under extreme conditions: Building surrogate models with machine learning

Monday, November 22, 2021 1:30 PM (1h 40m)

The accurate numerical treatment of matter under extreme conditions is crucial for the understanding of important physical phenomena such as radiation damage in fusion reactor walls, or planetary interiors. Yet, such simulations are unfeasible with state-of-art methods, e.g., density functional theory (DFT) if performed at large length and time scales, due to unfavorable scaling behavior. One possible route to mitigate these scaling issues are machine-learning based surrogate models; DFT data is used to calculate models that allow access to the same quantities of interest a DFT simulation would, at drastically reduced computational cost. CASUS (in cooperation with SNL and ORNL) develops a framework called "Materials Learning Algorithms" (MALA), drawing on which DFT surrogate models can easily be created and applied. Here we present an overview of MALA and recent results, such as size transferability and automated model construction.

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Session Classification: Poster Session 1

Contribution ID: **51** Type: **Poster**

Fermi surfaces of the chiral topological semimetal PtGa with maximal chern number

Monday, November 22, 2021 1:30 PM (1h 40m)

PtGa is a chiral topological semimetal with giant spin-split Fermi arcs with a maximal Chern number of four. We investigated the bulk Fermi surfaces of PtGa with angular-dependent de Haas-van Alphen (dHvA) measurements and band-structure calculations. Strong spin-orbit coupling leads to well separated spin-split bands. Eight bands cross the Fermi energy forming a multitude of Fermi surfaces resulting in intricate dHvA spectra. We were not able to assign all experimentally observed dHvA frequencies to the corresponding calculated extremal orbits, because of their considerable quantity and proximity. Yet, the experiment is in good agreement with the calculations confirming the topological character of PtGa.

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Presenter: SCHWARZE, Valentin (HZDR-HLD)

Session Classification: Poster Session 1

Contribution ID: **53** Type: **Poster**

Focused ion beam writing of color centers for quantum spin-photonic applications

Monday, November 22, 2021 1:30 PM (1h 40m)

Color centers and their optically interfaced spin read-out are one of the key building blocks for quantum information, quantum computing and quantum sensing [1,2]. The creation of atomic-scale spin centers as well as their integration into photonic structures such as micro-resonators, nanopillars and photonic crystals with sub-micrometer precision is of great importance for practical spin-photonic applications [3,4]. This work presents the controlled creation of quantum defect centers in silicon carbide with spin-photon interface using focused ion beam technologies. We also show the local writing of a novel color center in silicon, which has recently been demonstrated to exhibit single-photon emission in the optical telecom O-band [5,6], making it a promising candidate for quantum photonic applications.

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Session Classification: Poster Session 1

Contribution ID: **54** Type: **Poster**

Electrical and structural properties of NixGey thin films made by Magnetron sputtering and flash lamp annealing

Monday, November 22, 2021 1:30 PM (1h 40m)

Due to its higher charge carrier mobility compared to silicon, germanium belongs to the promising materials to surpass the physical limitations of the silicon based CMOS technology. For the integration of germanium into the CMOS process, the ohmic contact material with sufficiently low resistivity plays a crucial role. One of the promising candidates is nickel-germanide (NiGe) with a specific resistivity of $(13.5–22)\mu\Omega cm$. Those values are comparable with the nickel-silicides used in the CMOS process with electrical resistivities of around $17\mu\Omega cm$.

This work is focused on the formation process of NiGe films on different germanium layer morphologies, by the flash lamp annealing approach. Furthermore, the investigation on the Ni-Ge phase formation at different annealing temperatures was performed by grazing incidence X-ray diffraction and cross section transmission electron microscopy. The electrical properties were investigated by the application of four-point-probe, Hall effect and circular transfer length measurement techniques.

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Presenter: Mr BEGEZA, Viktor (HZDR)

Session Classification: Poster Session 1

Contribution ID: **55** Type: **Poster**

Towards a measurement of 14N(alpha, gamma)18F resonance strengths

Monday, November 22, 2021 1:30 PM (1h 40m)

The isotope ^{22}Ne is one of the main sources of neutrons for the astrophysical s-process of nucleosynthesis. It is linked via the reaction chain ^{14}N(α, γ)^{18}F(β^+)^{18}O(α, γ)^{22}Ne to the isotope ^{14}N, which is formed in stellar hydrogen burning. Selected resonances of the ^{14}N(α, γ)^{18}F reaction are studied at the Felsenkeller 5 MV accelerator by irradiating solid ^{14}N targets with a ^{4}He^{+} beam in an underground low-background setting. This measurement is part of the commissioning of the new internal radio-frequency ion source.

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Session Classification: Poster Session 1

Contribution ID: **56** Type: **Poster**

Measurement of the 3He(alpha,gamma)7Be gamma-ray angular distribution at the Felsenkeller shallow underground laboratory

Monday, November 22, 2021 1:30 PM (1h 40m)

The ^{3}He(α,γ)^{7}Be reaction plays a significant role in Big Bang nucleosynthesis, as well as solar fusion processes. Furthermore it affects the predicted solar ^{7}Be and ^{8}B neutrino fluxes as well as the nucleosynthesis of primordial ^{7}Li.
A measurement of the γ-ray angular distribution may enable a better comparison between several experimental data sets at E$= 0.7 - 1.3$ MeV and a unique data set from the LUNA collaboration at E$= 0.09$ MeV $- 0.13$ MeV. Therefore the ^{3}He(α,γ)^{7}Be reaction is currently being studied with the 5 MV Pelletron accelerator at the Felsenkeller shallow underground facility. The long-term focus lies on the measurement of the γ-ray angular distribution between $E_{\mathrm{cm}} \approx 0.5 - 1.3$ MeV.
In addition, the activated samples are counted offline. This newly installed counting setup contains a large HPGe detector (163 $\%$ relative efficiency) in a sophisticated shielding consisting of active and passive components. First results of this ongoing campaign will be summarized.

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Session Classification: Poster Session 1

Contribution ID: **58** Type: **Poster**

The possibility of spray coating of lignin and characterization of the thin film

Monday, November 22, 2021 1:30 PM (1h 40m)

Lignin is a binding agent in wood and very promising regarding the sustainable development of new bio-based applications. There is a rising awareness to invent and use environmentally friendly polymeric alternatives. Therefore, three different lignins were tested for spray coating. The lignin was dissolved in two different solvents, aceton and tetrahydrofuran. The structure and morphology as well as the crystallinity of the lignin thin films were investigated by using grazing incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS). By using atomic force microscopy, the surface morphology and film thickness were characterized. The main goal is to transfer the multifunctionality of lignin in a plant to novel materials and to discover new applications for the mainly considered waste product. In order to accomplish the goals, the characterization of the still unknown molecular and nanoscale arrangement of lignin in thin films via X-ray is of interest.

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Presenter: SNOKE, Sophie (DESY, Lignopure, TUHH)

Session Classification: Poster Session 1

Contribution ID: **59** Type: **Poster**

Rare earth induced ferroelectric-ferromagnetic multiferroicity in PrMn2O5 under strong magnetic field

Monday, November 22, 2021 1:30 PM (1h 40m)

Spin-driven ferroelectricity (SDFE) observed in some frustrated magnets is a crucial phenomenon paving the way towards next-generation data storage technology. In this context, investigation on the RMn2O5 (R = Bi, rare-earth) multiferroics is quite important as they show SDFE with strong magnetoelectric coupling. Interestingly, in contrast to all other members, PrMn2O5 does not show any SDFE when magnetically ordered. However, using the high-field electric-polarization tech-nique up to 45 T, we have found that this exceptional candidate undergoes a spin driven multifer-roic phase under strong magnetic field. High-field x-ray magnetic circular dichroism study shows that this ferroelectricity emerges from and directly couples to the ferromagnetic component of the Pr3+ moments. Experimental observations along with our theoretical calculations reveal that this unusual ferroelectric-ferromagnetic combination stabilizes through the exchange-striction mech-anism solely driven by a 3d-4f coupling, as opposed to the other RMn2O5 members with 3d-3d driven ferroelectric antiferromagnetic-type conventional type-II multiferroicity.

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Session Classification: Poster Session 1

Contribution ID: **60** Type: **Poster**

Crystallization in supercooled atomic liquids

Monday, November 22, 2021 1:30 PM (1h 40m)

Freezing of a liquid is a ubiquitous change of state, but many aspects of this phase transition are still poorly understood. Crystallization is classically viewed as a two-steps process. Thermal fluctuations in the supercooled liquid — that is, below its melting point — trigger the spontaneous formation of a small, localized nucleus of the new ordered phase, which subsequently grows to macroscopic dimensions. However, many details of the process still lack an adequate microscopic understanding. Here we combine x-ray scattering at the European X-ray Free-Electron Laser with atomic liquid jets as a powerful approach to the study of the early stages of crystallization in supercooled liquids, addressing the problem of the inherently stochastic nature of the crystal nucleation process as no a priori knowledge of the spatial and temporal coordinates of the spontaneous solid formation is in general available. These experiments promise to provide benchmarks for current theories of crystallization.

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Session Classification: Poster Session 1

Contribution ID: **61** Type: **Poster**

Magnetocaloric effect in the Laves-phase $Ho_{1-x}Dy_xAl_2$ family in high magnetic fields

Monday, November 22, 2021 1:30 PM (1h 40m)

Hydrogen has the largest gravimetric energy density among all chemical fuels. At the same time, the density of gaseous H_2 is extremely low, which makes its liquefaction necessary for transport purposes. Magnetocaloric materials have the great potential to revolutionize gas liquefaction to make liquid hydrogen more competitive as fuel. In this work, we investigate a series of Laves-phase materials regarding their structural, magnetic, and magnetocaloric properties in high magnetic fields. The three compounds $HoAl_2$, $Ho_{0.5}Dy_{0.5}Al_2$, and $DyAl_2$ are suited for building a stack for cooling from liquid-nitrogen temperature (77 K) down to the boiling point of hydrogen at 20 K. This is evident from our direct measurements of the adiabatic temperature change in pulsed magnetic fields, which we compare with calorimetric data measured in static fields. With this methodology, we are now able to study the suitability of magnetocaloric materials down to low temperatures up to the highest magnetic fields.

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Session Classification: Poster Session 1

Contribution ID: **62** Type: **Poster**

Fiber-integrated, high-repetition-rate water window soft X-ray source

Monday, November 22, 2021 1:30 PM (1h 40m)

Bright, coherent soft X-ray sources with photon energies within the water window (284-543 eV) are highly interesting for applications in spectroscopy or imaging. So far, these sources are based on large-scale facilities like synchrotrons and FELs, or realized through high-order harmonic generation, driven by high-peak-power laser systems with kHz repetition rate. In this work, we demonstrate nonlinear self-compression of pulses from a 100 kHz-repetition-rate 2 μm fiber laser, combined with phase-matched high-order harmonic generation in the same gas-filled hollow-core fiber. The intensity enhancement associated with the temporal pulse compression results in moderate requirements for the driving laser energy and pulse duration, which makes this approach highly interesting in the context of user-access and power-scaling. At the carbon K-edge (284 eV), the source generates a photon flux >106 photons/s/eV. To demonstrate the application relevance of this work, first proof-of-principle near absorption edge X-ray fine structure spectroscopy measurements in mylar are performed.

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Presenter: GEBHARDT, Martin (FSU Jena)

Session Classification: Poster Session 1

Contribution ID: **64** Type: **Poster**

Unconventional magnetism in the $RE_3Fe_3Sb_7$ spin system

Monday, November 22, 2021 1:30 PM (1h 40m)

Here we present a detailed magnetization and electrical-transport study of novel $RE_3Fe_3Sb_7$ com-pounds. We find a number of spontaneous magnetic phase transitions in a wide temperature range and a pronounced magnetic anisotropy. $RE_3Fe_3Sb_7$ shows an emergent spontaneous magnetiza-tion in zero field and a kink in the temperature-dependent resistivity at the spin-reorientation transition SRT. In the ground state, $RE_3Fe_3Sb_7$ displays a large uniaxial magnetic anisotropy that changes to planar at SRT. Our pulsed field magnetization measurements indicate a monotonic in-crease beyond 56 T, where the magnetization does not yet saturate. Our neutron scattering results reveal an unusual antiparallel alignment of Pr and Fe magnetic moments. In addition, XMCD mea-surements in pulsed magnetic fields up to 28 T indicate a continuous rotation of the Nd moment towards the Fe moment.

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Session Classification: Poster Session 1

Contribution ID: **65** Type: **Poster**

The BARB project (Biomedical Applications of Radioactive ion Beams)

Monday, November 22, 2021 1:30 PM (1h 40m)

Range uncertainties remains the main physical curbs of particle therapy. The use of radioactive ion beams for simultaneous treatment and online range verification using PET can help to overcome this limitation. Up to know, challenging production and low intensities have discouraged their clinical application. However, thanks to the accelerator developments in FAIR-Phase-0, it is now possible to produce at GSI (Darmstadt) radioactive ion beams with intensities high enough to treat a tumor in an animal model.
In this context, the BARB ERC AdG at GSI has the goal to assess the technical feasibility and advantages of 10,11C and 14,15O beams in preclinical studies. BARB is a large collaboration involving two FAIR pillars (APPA and NuSTAR) and universities (LMU and UMCG). Here we present the project together with some preliminary experimental and simulation results.

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Session Classification: Poster Session 1

Contribution ID: **66** Type: **Poster**

Swift heavy ions induced degradation of mechanical properties of graphitic materials

Monday, November 22, 2021 1:30 PM (1h 40m)

In high-intensity ion accelerators graphitic materials are an excellent choice for beam exposed components such as targets, beam dumps or collimators. Structural integrity and resilience to pulsed beams are required for safe operation of these devices. Irradiation induced hardening, in-crease of Young's modulus or embrittlement might lead to failure. Isotropic graphite and carbon fibre reinforced carbon were irradiated at the M Branch beamline at the UNILAC accelerator at GSI with C, Ca, Xe, Sm, Au, Bi and U ions in the GeV energy range to fluences between 1e11 and 2e14 ions/cm². Microindentation reveals large changes of Young's modulus by up to 300 % and an in-crease in hardness by more than 1000 %. Raman spectroscopy indicates a beam induced allotropic transformation of graphite to a structure similar to glassy carbon consisting of non-six-membered rings.

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Session Classification: Poster Session 1

Contribution ID: **68** Type: **Poster**

Spectroscopic micro-imaging with off-axis zone plates

Monday, November 22, 2021 1:30 PM (1h 40m)

Soft x-ray spectroscopies usually measure the average signal from the illuminated spot on the sample. This restricts the obtainable information if the sample is inhomogeneous (because of electronic domain formation or micro-patterning). Here, we demonstrate the commissioning of an experimental setup, build around an off-axis Fresnel zone plate, which enables parallel imaging of millimeter fields of view in x-ray absorption spectroscopy and resonant elastic and inelastic x-ray scattering with a spatial resolution down to 1.8 µm. The zone plate between sample and detector disperses x-rays scattered from the sample and also images the sample along the direction perpendicular to the dispersion. For quantum materials research for example, this setup enables novel studies of complex domain structures that may evolve in time which would be inaccessible through scanning methods. Novel insights into pinning and fluctuation dynamics are expected.

Reference: J. O. Schunck et al. Optica 8(2), 2021

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Presenter: SCHUNCK, Jan (DESY - FS FLASH)

Session Classification: Poster Session 1

Contribution ID: **69** Type: **Poster**

Measurement-Protocol Dependence of the Magnetocaloric Effect in Heusler Alloys. A pulsed magnetic field study.

Monday, November 22, 2021 1:30 PM (1h 40m)

Thermal hysteresis is a critical issue for the performance of magnetocaloric materials. Specifically, in the case of Heusler alloys that undergo a first-order magnetostructural transition, thermal hys-teresis, intrinsic of the transition, not only lead to irreversible effects, but to magnetocaloric prop-erties that highly depend on the measurement protocol at which they are obtained, for instance, whereas the initial temperature is approached on cooling or on heating. Consequently, the temper-ature dependent adiabatic temperature change (ΔTad) of Heusler alloys exhibit, likewise, thermal hysteresis.
In this work, we present the example of the Heusler alloys Ni-Co-Mn-Sb and Ni-Cr-Mn-In. Direct measurements of ΔTad were performed in pulsed magnetic fields at the Dresden High Magnetic field laboratory, HLD-EMFL, following different measurement protocols.

Primary authors: SALAZAR, Catalina (HLD-HZDR); BYKOV, Eduard (HLD-HZDR); NIEHOFF, Timo (HLD-HZDR); STRAßHEIM, Marc (HLD-HZDR); WOSNITZA, Jochen (HLD-HZDR); Dr GOTTSCHALL, Tino (HLD-HZDR)

Presenter: SALAZAR, Catalina (HLD-HZDR)

Session Classification: Poster Session 1

Contribution ID: **71** Type: **Poster**

A table-top Soft X-ray beamline for transient absorption experiments in liquid phase

Monday, November 22, 2021 1:30 PM (1h 40m)

Attosecond transient absorption spectroscopy, in particular when performed in the water window spectral range, offers the possibility of studying the electronic dynamics of biologically relevant molecules in their physiological environment (liquid phase), with the advantage of site-selectivity. In this work we report the development of an attosecond Soft X beamline which combines high harmonic generation with a liquid jet molecular source for aqueous phase experiments. The beamline is driven by a two-stages optical parametric source, which produces few-optical-cycle multi-mJ CEP-stable 1.8 μm carrier wavelength pulses. Furthermore, we present the construction of a microjet source able to generate stable liquid sheets, which are tunable in thickness from over 1 μm down to less than 20 nm. The advantage of microjets consists in a high photon transmission across the spectrum and in a simultaneous containment of pulse dispersion and sample damaging, opening the way for applications in infrared, X-ray and electron spectroscopies.

Primary author: GIOVANNETTI, Gaia (FS-ATTO CFEL DESY)

Presenter: GIOVANNETTI, Gaia (FS-ATTO CFEL DESY)

Session Classification: Poster Session 1

Contribution ID: **72** Type: **Poster**

Magnetocaloric effect and complex magnetic structure of Tb3Ni measured in pulsed fields

Monday, November 22, 2021 1:30 PM (1h 40m)

The magnetocaloric effect is a promising pathway towards a more efficient and environmentally friendly cooling and gas liquification and, therefore, triggered a vibrant research field. Compounds of the intermetallic family R3TM (R = Gd, Dy, Tb; TM = Co, Ni) had shown very interesting mag-netocaloric and magnetic properties. In this poster we present the magnetization data and magne-tocaloric properties in high pulsed magnetic fields in a single crystal of the compound Tb3Ni. The magnetic characterization data revealed a very complex phase diagram with temperature- and field-induced phase transitions suggesting a change from a conventional to an inverse magnetocaloric effect at low temperatures. In pulsed fields up to 50 T, we could confirm the complex behavior of Tb3Ni and with this, we can better understand its magnetic structures.

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Session Classification: Poster Session 1

Contribution ID: **191** Type: **Invited Talk**

Enabling ultra-intense laser experiments at HiBEF at EuXFEL

Monday, November 22, 2021 3:10 PM (20 minutes)

Presenter: LASO GARCIA, Alejandro (Helmholtzzentrum Dresden-Rossendorf(HZDR))

Session Classification: Session C

Contribution ID: **18** Type: **Invited Talk**

Surface Defects in Supercrystals of Caesium Lead Halide Perovskite Nanocrystals Revealed by Nanodiffraction

Monday, November 22, 2021 3:30 PM (20 minutes)

We exploited spatially-resolved X-ray nanodiffraction to study the structure of supercrystals of self-assembled caesium lead halide perovskite nanocrystals.[1] Analysis of the Bragg peaks in both small- and wide-angle scattering at each spatial point revealed a loss in structural coherence, an increasing atomic misalignment between adjacent nanocrystals, and growing compressive strain near the surface of the supercrystals. Comparison with the results of spatially-resolved fluorescence spectroscopy and lifetime measurements indicated an effect of the surface defects on the fluorescence properties of the supercrystals. Such surface defect-related optical properties extend the postulated analogy between atoms and nanocrystals as so-called quasi-atoms.

References

1. Lapkin, D. et al. (2021) (submitted). arXiv:2109.05502

Primary authors: LAPKIN, Dmitry (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Mr KIRSCH, Christopher (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Mr HILLER, Jonas (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Dr ANDRIENKO, Denis (Max Planck Institute for Polymer Research, Mainz, Germany); Ms ASSALAUOVA, Dameli (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Dr BRAUN, Kai (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Dr CARNIS, Jerome (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Dr KIM, Young Yong (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Dr MANDAL, Mukunda (Max Planck Institute for Polymer Research, Mainz, Germany); Dr MAIER, Andre (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Prof. MEIXNER, Alfred J. (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Dr MUKHARAMOVA, Nastasia (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Prof. SCHEELE, Marcus (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Prof. SCHREIBER, Frank (Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany); Dr SPRUNG, Michael (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany); Mr WAHL, Jan (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Ms WESTENDORF, Sophia (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany); Dr ZALUZHNYY, Ivan A. (Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany); Prof. VARTANYANTS, Ivan A. (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany)

Presenter: LAPKIN, Dmitry (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany)

Session Classification: Session C

Contribution ID: **25** Type: **Invited Talk**

Study of preplasma properties using time-resolved reflection spectroscopy

Monday, November 22, 2021 3:50 PM (20 minutes)

The state and properties of the preplasma prior to the arrival of the peak of the laser irradiation is critical to understanding relativistic laser plasma interactions. The spectral properties of a re-flected laser pulse after the interaction with the plasma, where holeboring has a predominant role, can be used to gain insights about the conditions of the preplasma itself. We developed an ana-lytical model, describing the non-relativistic temporal evolution of the holeboring velocity, for an arbitrary overdense plasma density and laser intensity profile, which is confirmed with the help of two-dimensional particle-in-cell simulations. The influence of the holeboring dynamic on the reflected laser pulse can be measured and the corresponding spectral modulation can be used to determine the preplasma properties in laser-plasma interaction experiments.

Primary authors: HORNUNG, Johannes (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI)); ZOBUS, Yannik; RÖDER, Simon (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI)); KLEINSCHMIDT, Annika (GSI, Darmstadt); BERTINI, Denis (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI)); ZEPF, Karl Matthäus (GSI, Darmstadt); BAGNOUD, Vincent (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Presenter: HORNUNG, Johannes (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classification: Session C

Contribution ID: **2** Type: **Invited Talk**

Accelerator-based generation of space radiation @ GSI/FAIR

Monday, November 22, 2021 4:10 PM (20 minutes)

Risks for man and machine associated with the chronic exposure to the highly energetic ions of the galactic cosmic rays or sporadic solar particle events are one of the main obstacles for the manned exploration of the solar system. High energy particle accelerators, like GSI/FAIR, are a necessity to study the deleterious effects induced by the broad range of ion species and energies of the space radiation environment. However, serialized experimental studies using individual ion species and energy combinations, as typically performed at particle accelerators, cannot be used to study all relevant effects induced by the complex radiation environment in space. Therefore, GSI/FAIR, supported by ESA, started the development of an advanced space radiation simulator. High energy iron beams are passively modulated by sets of complex modulators to closely mimic the radiation environment for different space mission scenarios.

Primary author: SCHUY, Christoph (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Presenter: SCHUY, Christoph (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classification: Session C

Contribution ID: **23** Type: **Invited Talk**

Impact of radiation quality on the DNA double-strand break repair pathway choice in particle radiotherapy – an in vitro study comparing carbon, protons and photons at GSI

Monday, November 22, 2021 4:30 PM (20 minutes)

Beside conventional photon irradiation, charged particles and especially protons are employed as major strategies to treat tumors. In addition to their advantageous depth dose profiles, the heavier charged particles offer the benefit of a higher biological effectiveness (RBE) at the same physical dose. This high RBE is mainly based on the induction of clustered DNA double-strand breaks (DSBs) that some authors believe to be largely repaired by homologous recombination (HR). Although protons are considered as relatively sparsely ionizing irradiation, recent research indicated that repair of the proton induced DSBs mainly relies on HR. This is distinct from photon irradiation, which requires non-homologous end-joining (NHEJ) for repair. These differences might have consequences for combinatorial treatments and patient stratification.
In our study, we characterize the utilization of different DNA repair pathways in a cell-cycle dependent manner by using live cell imaging as main approach. Our goal is to identify the DNA repair pathways elicited by different radiation qualities to tweak targeted drug therapy in combination with X-ray and particle radiotherapy.

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Presenter: KRATZ, Katja (GSI Helmholtzzentrum für Schwerionenforschung GmbH (GSI))

Session Classification: Session C

Contribution ID: **192** Type: **Invited Talk**

CCA Radiation Research

Tuesday, November 23, 2021 9:00 AM (20 minutes)

Presenter: DURANTE, Marco (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classification: Session D

Contribution ID: **52** Type: **Invited Talk**

Probing the dynamical local structure of isolated to solvated proteins

Tuesday, November 23, 2021 9:20 AM (20 minutes)

Proteins are the building blocks of life and it is important to understand how exactly their physical properties are responsible for their functionality and responses to stressors. A very suitable method is to study isolated biomolecules with cutting-edge mass spectrometry techniques at advanced light sources to unravel their intrinsic properties, i.e. in an environment-free and controlled chemical state. In particular, Near-Edge X-ray Absorption Mass Spectrometry (NEXAMS), which is an action-spectroscopy technique based on fragment-resolved absorption upon resonant photoexcitation of core atomic levels, has been of growing interest in recent years for investigating the spatial and electronic structure of biomolecules.
In this talk, I will present the latest results from NEXAMS studies on peptides and related molecules like porphyrins. Not only spatial and electronic structures, but also damage processes, site-selective dissociation, and orbital-dependent deexcitation pathways are discussed, and an outlook on solvation studies is given.

Primary author: BARI, Sadia (DESY)

Presenter: BARI, Sadia (DESY)

Session Classification: Session D

Contribution ID: **19** Type: **Invited Talk**

Probing microsecond dynamics in liquids and soft matter at European XFEL

Tuesday, November 23, 2021 9:40 AM (20 minutes)

The European XFEL as a megahertz hard X-ray Free-Electron Laser source uniquely enables such experiments via taking series of diffraction patterns at repetition rates of up to 4.5 MHz. Here, we demonstrate X-ray photon correlation spectroscopy (XPCS) with submicrosecond time resolution of soft matter samples making use of the MHz repetition rate of the European XFEL. We show that the XFEL driven by a superconducting accelerator provides unprecedented beam stability within a pulse train. This allowed us to perform microsecond sequential XPCS experiments probing equilibrium and nonequilibrium diffusion dynamics of nanoparticles in water. We find nonlinear heating on microsecond timescales with dynamics beyond hot Brownian motion and superheated water states up to 445 K persisting up to 100 μs at high fluences. We further show that it is possible to correctly identify the dynamical properties of soft matter samples, both for stationary samples and for systems driven by XFEL pulses.

Primary author: LEHMKÜHLER, Felix (DESY)

Presenter: LEHMKÜHLER, Felix (DESY)

Session Classification: Session D

Contribution ID: **82** Type: **Invited Talk**

Functional biomaterial-based hybrid materials SERS applications

Tuesday, November 23, 2021 10:00 AM (20 minutes)

Metal nanoparticles (MNPs) composites have attracted growing interest due to their structure-dependent properties. However, the control over the assembly of MNPs with tailored morphology and crystallinity remains a challenge. Bio-templated fabrication of MNP layers is a promising route for transferring the ordering of templates into the MNP layers, among which cellulose nanofibril (CNF) is a promising candidate. Herein, we used silver (Ag) and titanium dioxide (TiO2) nanoparticles (NPs) to demonstrate the templating efficiency of CNFs. Through layer-by-layer spray-coating, we found that CNFs contribute to the uniform distribution of AgNP layer with tailarable wettability [1]. Additionally, through modulation of the template morphology of CNFs and the crystallinity of TiO2 via atomic layer deposition, TiO2/CNF thin films achieved a high enhancement factor of 1.8 × 106 in terms of semiconductor metal oxide-based surface-enhanced Raman scattering substrates [2].
[1] ACS Appl. Nano Mater. 2021, 4, 503-513
[2] Adv. Funct. Mater. 2021, 2108556

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Presenter: CHEN, Qing (DESY)

Session Classification: Session D

Contribution ID: **50** Type: **Invited Talk**

High-resolution imaging of small molecules using laser-induced electron diffraction

Tuesday, November 23, 2021 10:20 AM (20 minutes)

We will discuss opportunities for high-spatial-resolution imaging of the structural dynamics of small molecules opened up by laser-induced electron diffraction (LIED). We will introduce the method in the context of classical coherent-diffractive-imaging approaches and discuss its merits and challenges in the context of our current progress toward precision measurements, i.e., to the determination of bond lengths to within 5 pm. This will lead to a discussion of the potential of imaging ultrafast structural dynamics of chemical processes in molecular quantum systems using pump-probe techniques.

Primary author: ROBINSON, Matthew (CFEL)

Co-author: Prof. KÜPPER, Jochen (CFEL)

Presenter: ROBINSON, Matthew (CFEL)

Session Classification: Session D

Contribution ID: **7** Type: **Invited Talk**

Probing Inner-Shell-Ionization-Induced Femtosecond Structural Dynamics of Water Molecules with X Rays and Simulations

Tuesday, November 23, 2021 11:00 AM (20 minutes)

We have exposed isolated water molecules to ultra-short and ultra-intense x-ray pulses from a free-electron laser and detected momenta of all produced ions in coincidence. The break-up of the molecule triggered by core-shell photoionization and Auger decay could be traced by analyzing the momenta of highly charged ion momenta created via absorption of multiple x-ray photons. By combining the experimental data with our theoretical modeling, we can image the dissociation dynamics of water in unprecedented detail and uncover fundamental dynamical patterns relevant for the radiation damage in aqueous environments.

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Presenter: INHESTER, Ludger (Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY)

Session Classification: Session E

Contribution ID: **186** Type: **Invited Talk**

Exploring the Femtosecond Dynamics of Polycyclic Aromatic Hydrocarbons Using XUV FEL Pulses

Tuesday, November 23, 2021 11:20 AM (20 minutes)

Satellite infrared measurements show signatures of aromatic vibrations in practically every corner of the universe, attributed to polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM). These PAHs account for up to 20% of carbon in space and have long been proposed as carriers of the Diffuse Interstellar Bands and Unidentified Infrared Bands. Utilising XUV pulses from the Free-Electron-Laser FLASH replicates some of the harsh radiation of the interstellar medium and allows a detailed insight into the various molecular processes occurring after the initial photoionisation. Our experiments investigate the ultrafast relaxation and fragmentation of PAHs in a pump-probe regime.

Primary author: LEE, Jason (Deutsches Elektronen-Synchrotron DESY)

Presenter: LEE, Jason (Deutsches Elektronen-Synchrotron DESY)

Session Classification: Session E

Contribution ID: **11** Type: **Invited Talk**

Ultrafast real-time dynamics during Photocatalysis

Tuesday, November 23, 2021 11:40 AM (20 minutes)

Studies of photocatalytic reactions on TiO2 are instrumental to the development of technology used for self-cleaning surfaces and for air and water purification. We utilize femtosecond X-ray laser pulses synchronized with an optical laser to directly follow the reaction dynamics of the photooxidation of CO on the anatase TiO2(101) surface. Our time-resolved soft X-ray photoemission spectroscopy results allow us to elucidate the mechanism of oxygen activation and provide evidence of ultrafast timescales. The reaction takes place between 1.2 - 2.8 (± 0.2) ps after irradiation with an ultrashort laser pulse, resulting in CO2. No intermediate species were observed on a picosecond time scale. Theoretical calculations predict that the reaction can be initiated following the formation an O2-TiO2 charge-transfer complex. This allows the reaction to take place following laser illumination at a photon energy of 1.6 eV (770 nm), following the direct transfer of electrons from TiO2 to physisorbed O2.

Primary author: WAGSTAFFE, Michael

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Presenter: WAGSTAFFE, Michael

Session Classification: Session E

Contribution ID: **115** Type: **Invited Talk**

Molding of Light - Tunable IAPs from Optical Waveform Synthesizers & Pulse Compression at its Limits

Tuesday, November 23, 2021 12:00 PM (20 minutes)

This contribution covers two state-of-the-art approaches for generating and shaping ultrashort light pulses: optical waveform synthesizers and extreme post-compression using multi-pass cells. The coherent synthesis of different phase-stable pulses, obtained via optical parametric amplifiers, enables the generation of customizable electromagnetic waveforms with sub-cycle duration and mJ-level energy. These tailored light-fields offer great capabilities for controlling and steering electron trajectories in strong-filed driven processes enabling the creation of isolated attosecond pulses whose central energy, spectral bandwidth and duration are widely tunable. As alternative to parametric amplification, high-power Ytterbium-based lasers, which are typically used as pump-sources for parametric amplifiers, can be directly post-compressed. This way, ultrashort pulses can be generated with very high efficiency. In particular, novel multi-pass cell-based post-compression units offer great prospects for high average power, few-cycle pulse generation with applications ranging from free-electron laser pump-probe spectroscopy over high-harmonic sources to plasma acceleration.

Primary authors: HEYL, Christoph M. (DESY); ROSSI, Giulio Maria (Deutsches Elektronen-Synchrotron)

Presenter: ROSSI, Giulio Maria (Deutsches Elektronen-Synchrotron)

Session Classification: Session E

Contribution ID: **176** Type: **Invited Talk**

High-purity X-ray polarimetry

Tuesday, November 23, 2021 12:20 PM (20 minutes)

High-precision X-ray polarimetry has made great progress in the last year to realize the detection of vacuum birefringence. On the one hand, the polarization purity could be further increased, and on the other hand, it was possible to focus and recollimate the high-precision polarized beam with X-ray lenses without destroying the purity. For this purpose, different lens materials were investigated at PETRA III and the setup with X-ray lenses was tested for the first time at the European XFEL.

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Presenter: SCHMITT, Annika Tamara (Friedrich-Schiller-Universität Jena)

Session Classi ication: Session E

Contribution ID: **73** Type: **Poster**

Isolated attosecond pulses generated by synthesized sub-cycle waveforms

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The generation of ultrashort and intense laser pulses shorter than an optical cycle, hence sub-cycle pulses, is one major quest in contemporary ultrafast laser science. Tailored sub-cycle waveforms can give rise to the production of bright isolated attosecond pulses in the extreme ultraviolet and soft x-ray spectral regions via high-harmonic generation. By means of time-resolved spectroscopic techniques, isolated attosecond pulses can thus allow studying underlying electronic dynamics of chemically- and biologically-relevant systems at their natural timescales. We experimentally proved the coherent combination of two phase-stable, optically parametrically-amplified few-cycle laser pulses in the infrared range (covering together from 650 nm to 2.2 μm) to create customized, high-energy laser pulses reaching pulse durations down to 0.6 optical cycles. We generate isolated attosecond pulses that exhibit spectral and temporal tunability upon modifications of the synthe-sized waveform. Using the attosecond streaking technique, the temporal profile of the synthesized waveforms and attosecond pulses is retrieved.

Primary authors: SILVA TOLEDO, Miguel Angel (Deutsches Elektronen-Synchrotron); YANG, Yudong (Deutsches Elektronen-Synchrotron); MAINZ, Roland E. (Deutsches Elektronen-Synchrotron); ROSSI, Giulio Maria (Deutsches Elektronen-Synchrotron); SCHEIBA, Fabian (Deutsches Elektronen-Synchrotron); KEATH-LEY, Phillip D. (Massachusetts Institute of Technology); CIRMI, Giovanni (Deutsches Elektronen-Syn-chrotron); KÄRTNER, Franz X.

Presenter: SILVA TOLEDO, Miguel Angel (Deutsches Elektronen-Synchrotron)

Session Classi ication: Poster Session 2

Contribution ID: **74** Type: **Poster**

Phase evolution of Te-hyperdoped Si upon furnace annealing

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Silicon doped with Tellurium (Te), a deep level impurity, at concentrations higher than the solid solubility limit (hyperdoping), has been achieved by ion-implantation and nanosecond pulsed laser melting. The resulting materials exhibit a strong sub-bandgap optical absorption, showing potential for room-temperature broadband Infrared photodetectors. As a thermodynamically metastable system, an impairment of the optoelectronic properties in hyperdoped Si materials occurs upon subsequent high-temperature thermal treatment. The substitutional Te atoms that cause the sub-bandgap absorption are removed from the substitutional sites to form Te-related complexes. In this work, we explore the phase evolution and the electrical deactivation of Te-hyperdoped Si layers upon furnace annealing through the analysis of optical and microstructural properties as well as positron annihilation lifetime spectroscopy. Particularly, Te-rich clusters are observed in samples annealed at temperatures reaching 950 ℃ and above. Combined with polarized Raman analysis and transmission electron microscopy, the observed clusters are suggested to be Si2Te3.

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Session Classi ication: Poster Session 2

Contribution ID: **75** Type: **Poster**

Modification of epitaxial La0.6Sr0.3CoO3-δ thin films by ion irradiation

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Perovskite oxides exhibit rich physics related to ionic defects. In particular, defect concentration and distribution alter the lattice parameters and affect the competitive interplay between strongly correlated electrons, enabling numerous applications, including sensors, catalysts, and memristive devices. In this work, helium-implantation is demonstrated as a fast, low-temperature tool to modulate the vacancy profiles in epitaxial La0.6Sr0.4CoO3-δ thin films. Not only a significant lattice expansion solely along the out-of-plane direction is observed, but also a distinct change in physical properties is evidenced. By proper tuning of the implantation parameters, an enhanced resistivity up to several orders of magnitude is achieved at room temperature. These results offer a new playground for the optimization of oxide-based spintronic and electronic devices.

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Presenter: ZHOU, Yunxia

Session Classification: Poster Session 2

Contribution ID: **76** Type: **Poster**

Interfacial control of phase transitions in magnetic oxide heterostructures through electric field for magnetic switching

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Tuning magnetic oxide phases via redox reactions across their heterointerfaces makes them useful for spintronic and memristive device applications. With controlled film-substrate interfaces and using small electric field, oxidation/reduction reaction occurs which leads to a reversible phase transition. In this work, we achieve magnetic switching of Fe3O4/Nb:SrTiO3 heterosturctures by applying electric field. We grow Fe3O4 films with different growth temperatures by pulsed laser deposition. The quality of the magnetite films is checked by different techniques e.g. AFM and XMCD. Using magnetometry, we detect the Verwey transition which is a strong indicator of the oxygen content in the Fe3O4 films. We observe a strong change in the Verwey transition with applied electric field. This can be explained by oxygen diffusion through the interface which leads to a reversible phase transition from Fe3O4(magnetite) to γ-Fe2O3(maghemite). Additionally, we investigate the structural transitions using x-ray diffraction (XRD) and insitu-wide angle scattering (WAXS).

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Session Classification: Poster Session 2

Contribution ID: **78** Type: **Poster**

Laser spectroscopy at storage rings

Tuesday, November 23, 2021 1:30 PM (1h 40m)

One of the research topics carried out at the Helmholtz Center for Heavy Ion Research in Darmstadt is high-precision laser spectroscopy studies in the magnetic storage rings. We are for example investigating the nuclear polarization by using the optical pumping effect at CRYRING@ESR. Preparations are presently ongoing at the ESR to measure the “nuclear clock” isomer transition utilizing the nuclear hyperfine mixing in 229Th89+ and to employ a new technique, called dielectronic recombination assisted laser spectroscopy, to measure the hyperfine splitting in lithium-like 209Bi80+. In this poster presentation, I will focus on the status of hyperfine spectroscopy measurements at the ESR to test bound-state strong-field QED.

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Session Classification: Poster Session 2

Contribution ID: **79** Type: **Poster**

Current developments on the GSI facility for ion irradiation of materials pressurized in diamond anvil cells

Tuesday, November 23, 2021 1:30 PM (1h 40m)

In the past decades, extensive research has demonstrated that under pressure, materials can have fascinating properties. In this poster, we present the high-pressure irradiation facility at GSI, where materials are simultaneously exposed to high static pressures and high energy heavy ion irradiation. Pioneering experiments at the SIS-18 accelerator at GSI revealed new effects such as the generation of new phases far from thermodynamic equilibrium or the stabilization of high pressure phases at ambient conditions. The experiments require compressing a miniaturized sample in a diamond anvil cell (DAC) and irradiate the cell with relativistic heavy ions of typically several tens of GeV kinetic energy. Monitoring beam-induced structural changes is provided by on-line analysis of the sample in the DAC by means of Raman spectroscopy. Specific challenges such as optimizing beam collimation and precise sample positioning will be discussed. The high-pressure station will be available for research groups from various disciplines.

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Session Classification: Poster Session 2

Contribution ID: **80** Type: **Poster**

Magneto Elastic Properties Of α-RuCl3 Probed By Ultrasound Under Hydrostatic Pressure

Tuesday, November 23, 2021 1:30 PM (1h 40m)

As a premier candidate for the quantum spin liquid (QSL) in the frame of the Kitaev model, a honeycomb material such as α-RuCl3 is of particular interest. Although α-RuCl3 exhibits an antiferromagnetic order below 7 K, it is handled as proximate to the QSL. The QSL is featured by its fractionalized quasiparticle excitations. A promising approach for investigations in this vein is the coupling between fractionalized quasiparticles and phonons. This is traceable in the attenuation coefficient and in the sound velocity of ultrasound. Our recent studies of the elastic properties of α-RuCl3 show a promising path to unveil the unconventional physics of the debated QSL phase. Here we present low temperature results of the sound velocity and attenuation at external magnetic fields and hydrostatic pressures. Observed anomalies in the acoustic properties and strong magnetoelastic couplings shed new light on the unconventional physics in this compound.

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Presenter: HAUSPURG, Andreas (HLD-HZDR)

Session Classification: Poster Session 2

Contribution ID: **81** Type: **Poster**

Spraying sustainable electrodes using cellulose and silver nanowires

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The use of environmentally friendly materials in future functional designs is as topical than ever. Cellulose nanofibrils (CNFs) are wood-based, lightweight, flexible, and strong, making them most suitable for the fabrication of sustainable composite materials. Furthermore, they are dissolvable in water and can therefore be sprayed easily. Using spray deposition, the preparation of thin, homogenous films of large scale and with an ultra-low roughness as well as their functionalization with e.g. nanoparticles is possible. In this study we use CNF as a sustainable template material for the fabrication of two different types of thin silver nanowire (AgNW) electrodes via spray deposition. We compare the structural and electrical properties of both types using SEM, AFM, grazing incidence small angle X-ray scattering (GISAXS), and conductivity measurements. We demonstrate the structural differences between both types and show the beneficial templating effects of CNF on the electronic properties of an AgNW network.

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Session Classification: Poster Session 2

Contribution ID: **84** Type: **Poster**

Improved predictions of biological effects after exposure to ion radiation with the Local Effect Model

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Radiobiological models for the prediction of effects after exposure to densely ionizing radiation are essential in various scenarios. On the one hand, they are successfully applied in cancer therapy treatments to optimize treatment plans for patients. On the other hand, they enable the prediction of hazardous effects after radiation accidents or during human space travel. Since 1997 the Local Effect Model (LEM) I has been clinically applied for the optimization of carbon ion treatment plans for cancer patients. Over the years, the model was further optimized leading to LEM IV, which is available since 2010. However, comprehensive model tests revealed a systematic underestimation of the biological effects after exposure to high energetic ions for LEM IV. In this work, the LEM V is presented, which enables an improved prediction for high energetic ions due to a new concept of including secondary electron spectra in the effect calculation after ion radiation.

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Session Classification: Poster Session 2

Contribution ID: **85** Type: **Poster**

The high brilliance laboratory X-ray diffractometer GALAXI: Results and Projects

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The high brilliance laboratory small angle X-ray scattering instrument GALAXI is used to investigate, on mesoscopic length scales, structural correlations in bulk materials or between objects deposited on a surface. Some results on the core-shell structure and self-organisation of nanoparticles as well as on the depth profile of a thin film heterostructure, obtained respectively by SAXS and GISAXS as well as XRR, will be displayed.
The device properties of thin film heterostructures crucially depend on the structure of the surface and interfaces, not only at the mesoscopic length scale but also at the interatomic length scale. We therefore aim at extending the instrument's capabilities towards grazing incidence wide-angle scattering (GIWAXS) and surface X-ray diffraction (SXRD). The eventual realisation of this project will be discussed, considering the wavelength distribution of the photons emitted by the source. First results from GALAXI used in the WAXS mode will also be displayed.

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Session Classification: Poster Session 2

Contribution ID: **86** Type: **Poster**

Data reduction in protein crystallography

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The amount of data measured during protein crystallography experiments is rather big and for serial crystallography (SX) it is simply huge – it can already exceed 2Pb per experiment. Therefore some data reduction strategy has to be applied. We propose to use combination of: non-hits rejection (saving only hits in "raw format"), rounding to integer numbers (where detectors allow), binning (for the cases when there minimum more than 10 pixels between Bragg peaks at the diffraction pattern) and in future using some additional lossy compression. But any of such methods have to be carefully tested, so the data quality is not reduced after the compression.

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Session Classi ication: Poster Session 2

Contribution ID: **87** Type: **Poster**

3D gold nanowire networks fabricated by ion-track nanotechnology as catalyst for methanol electro-oxidation

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Gold is a promising catalyst for multiple electrochemical reactions. Especially the use of nanostructured gold as catalyst has drawn much attention. In this poster we will present the synthesis of free-standing Au nanowire networks by ion-track technology and electrodeposition. The catalytical performance of the networks is studied for various wire diameters.
Polycarbonate foils are irradiated sequentially with GeV heavy ion beams from four directions at the UNILAC accelerator of GSI. Subsequent chemical etching of the ion tracks results in membranes with interconnecting nanochannels. Au nanowire networks are synthesized by potentiostatic electrodeposition. Nanowire growth rate and homogeneity are tuned by varying the deposition potential. After dissolving the polymer, the catalytic performance of the free-standing networks towards methanol oxidation is studied as a function of nanowire diameter. The results reveal high current densities and high catalytic activity of the networks, compare with a planar gold electrode.

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Session Classification: Poster Session 2

Contribution ID: **88** Type: **Poster**

Interferometric measurements for ultrashort UV pulses characterization

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Several groups have demonstrated the generation of few-fs ultraviolet (UV) pulses. However, the temporal characterization of such pulses is not a trivial task. The main issue is associated with the ultra-broadband nature of the UV spectrum, over which any dispersion needs to be avoided. In this regard, characterization techniques should be implemented in dispersion-free schemes. One of the candidates fulfilling this requirement is the fringe-resolved interferometric autocorrelation (FRIAC) method.

Here, we present the successful implementation of a second-order FRIAC approach for the characterization of ultrashort UV pulses generated by tripling a 10 fs infrared field in a neon medium. Two copies of the incident pulses are created using a reflective beam splitter formed by two intertwined comb-like mirrors. Each of them acts like a grating producing a clearly resolved diffraction pattern. Overlapping the single patterns spatially and temporally allows for recording the autocorrelation signal with interferometric contrast.

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Session Classi ication: Poster Session 2

Contribution ID: **89** Type: **Poster**

Single-stage post-compression of an Ytterbium fiber laser towards few-cycle regime

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Ytterbium-based laser systems are well known for their power scalability. However, they are mainly limited by their pulse duration which is in the order of few 100 fs to ps. Combining spectral broadening techniques with post-compression is a commonly employed path to overcome this limitation. Recently, nonlinear post-compression employing gas-filled Multipass Cells has evolved as an attractive solution providing high efficiency, compact setup sizes and excellent beam quality. Here we present our works towards reaching the few-cycle regime directly in a gas-based single-stage Multipass Cell. Our results show a compression of 150 fs pulse duration with ~230 uJ pulse energy down to sub-20 fs, giving a throughput of over 93%. The pulse duration achievable within a single compression stage can be pushed well beyond the current limit by employing dispersion-engineered dielectric mirrors to control the nonlinear spectral broadening.

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Session Classification: Poster Session 2

Contribution ID: **90** Type: **Poster**

Ultrathin hard magnetic coatings with perpendicular strong anisotropy by a spray deposition technique

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Hard magnetic SrFe₁₂O₁₉ nanoplatelets (5×50 nm²) and nanoblocks (7×20 nm²) with perpendicular magnetic moment orientation are self-ordered on silicon and flexible cellulose substrates from the surfactant-free colloids using layer-by-layer spray deposition. The uniform magnetic coatings of thickness controlled from a monolayer coverage up to the thickness of ~50 nm show preferred in-plane orientation of >80% for nanoplatelets and up to 75% of nanoblocks. Orientational ordering diminished on increasing film thickness. The high coercivity of the films of up to 5 kOe and high perpendicular anisotropy of M_{R⊠}/M_S»80% are provided with the proposed method. Application of the magnetic field during film deposition enables additional improvement in perpendicular magnetic anisotropy and the appearance of residual magnetization in the film of up to 0,6 M_S. Reducing the aspect ratio of magnetic particle shape (e.g., nanoblocks) allows forming of a semblance of an opal-like structure under the action of an external magnetic field.

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Session Classification: Poster Session 2

Contribution ID: **91** Type: **Poster**

Controllable generation and permeability of alginate/chitosan-based microcapsules for the encapsulation of liver cancer cells

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Cancer is a leading cause of death in the world. Traditional 2D cell culture systems are unable to simulate the microstructure, microenvironment, and some specific key functions of organs. Compared to 2D models, organoids as emerging 3D models can mimic key features of native organs such as gene and protein expression, metabolic function, and microscale tissue architecture. We used a fluidic cross-junction system to generate alginate/chitosan-based microcapsules for culturing liver cancer cells in Dulbecco's Modified Eagle Medium. The system can generate hundreds of microcapsules within a few minutes, enabling rapid and reliable analysis of microcapsule properties. We systematically investigated the effects of capsule diameter (200–1000 μm) and shell thickness (2–150 μm) on the permeability of microcapsules. Semipermeability of microcapsules, which is an important property for cancer cell culturing, was confirmed by monitoring the permeation of different fluorescent chemicals.

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Session Classi ication: Poster Session 2

Contribution ID: **92** Type: **Poster**

FIB microstructures of crystalline heavy-fermion metals studied in high magnetic fields and at low temperatures

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The heavy-fermion compound CeCoIn5 has attracted significant scientific interest in the past due to various intriguing physical properties, such as a d-wave superconducting ground state with Tc = 2.3 K, and an anisotropic electronic structure with peculiar field-induced changes. Below its Kondo-coherence temperature, TK = 30 K, CeCoIn5 exhibits perfect metallic behavior with very high conductivity. However, its resistivity is strongly anisotropic between the a and c direction. At magnetic fields larger than 20 T, additional transitions have been reported that resemble observations in other Ce-based heavy-fermion superconductors.
We performed high-precision magnetoresistance and Hall-effect measurements on micron-sized transport devices of CeCoIn5 in high magnetic fields (< 36 T) and low temperatures (> 30 mK). The devices were fabricated by focused ion beam (FIB) assisted micropatterning enabling reduced dimensions in order to improve on the detection signal. Our anisotropy studies provide new insights into the electronic properties of this versatile compound.

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Presenter: STIRNAT, Julia (HZDR)

Session Classification: Poster Session 2

Contribution ID: **93** Type: **Poster**

Transient negative thermal expansion in HgTe/CdTe heterostructures by heating transverse phonons

Tuesday, November 23, 2021 1:30 PM (1h 40m)

We investigate the transient negative thermal expansion of semimetallic HgTe and semiconducting CdTe heterostructures using synchrotron-based time-resolved X-ray diffraction. At $T = 20$ K, below the Debye temperature of both materials, the selective optical excitation of HgTe with an ultrashort near-infrared laser pulse leads to a rapid expansion of HgTe that is followed by a long lasting contraction. The CdTe substrate is compressed by the HgTe film expansion, and subsequently CdTe contracts due to thermally excited transverse phonon modes. This shows that negative thermal expansion is manifested on ultrafast timescales, consistent with the negative Grüneisen coefficient for transverse phonons in semiconducting materials with sphalerite crystal structure. At $T = 200$ K, above the Debye temperature of both materials, the expansion driven by longitudinal acoustic phonons is prevalent. We simulate the lattice dynamics in an elastic model where transient thermal stresses are calculated via heat diffusion based on equilibrium thermoacoustic properties.

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Session Classification: Poster Session 2

Contribution ID: **94** Type: **Poster**

Sub-3 nm Resolution 3D Diffractive Imaging of Anisotropic Gold Nanoparticles with Millions of Patterns using MHz XFEL Pulses

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Single particle imaging at x-ray free electron lasers (XFELs) has the potential to determine the structure and dynamics of single biomolecules at room temperature. Two major hurdles have prevented this potential from being reached, namely, the collection of sufficient high-quality diffraction patterns and robust computational purification to overcome structural heterogeneity. We report the breaking of both of these barriers using gold nanoparticle test samples, recording around 10 million diffraction patterns at the European XFEL and structurally and orientationally sorting the patterns to obtain better than 3-nm-resolution 3D reconstructions for each of four samples. With these new developments, integrating advancements in x-ray sources, fast-framing detectors, efficient sample delivery, and data analysis algorithms, we illuminate the path towards sub-nanometer resolution biomacromolecular XFEL imaging.

Ref: K. Ayyer+, P.L. Xavier+ et al. Optica, 8, 15-23, 2021 (+equal contribution)

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Session Classi ication: Poster Session 2

Contribution ID: **95** Type: **Poster**

Electrical characterization of highly doped germanium nanowires using Hall bar configuration

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Germanium (Ge) is the most compatible material with silicon-based complementary metal-oxide-semiconductor processes. Ge has a higher electron and hole mobility compared to Si, leading to improved device performance. Moreover, Ge nanowires (GeNWs) are promising nanostructures for future nano- and optoelectronics due to their unique properties. In this work, ion implantation of phosphorous followed by flash lamp annealing (FLA) operated in millisecond time scale were used to fabricate highly-doped n-type Ge layer on insulator. Raman spectroscopy and Rutherford backscattering spectrometry were performed to characterize the crystallinity of the Ge layers after FLA. Subsequently, doped GeNWs were fabricated using electron beam lithography and inductively coupled plasma reactive ion etching. Electrical characterization of the GeNWs was conducted using symmetric six-contact Hall bar configuration. The effect of nanowire width on transport parameters was investigated. Moreover, FLA was applied to fabricate NiGe alloy on a highly doped Ge layer for low-resistance ohmic contacts.

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Session Classi ication: Poster Session 2

Contribution ID: **96** Type: **Poster**

Bound-state beta decay of 205Tl

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Bound-state beta decay is an exotic decay mode in which the created electron remains bound in the ion. Obviously, this decay can proceed only in highly charged ions and is relevant for nucleosynthesis in stellar plasmas. This is an example of the interplay between atomic-, nuclear-, astro- and plasma physics. 205Tl is stable as neutral atom and becomes radioactive if all electrons are removed. The corresponding measurement was proposed more than 30 years ago and–owing to versatile capabilities of the storage ring ESR to manipulate ion beams–has now been successfully accomplished. The decay rate of 205Tl is needed to conclude on the termination of the s-process nucleosynthesis and on the possibility to use 205Tl as a Solar-neutrino detector. The measured decay rate is a factor of 2-5 smaller than predicted by theory. The experiment and the preliminary results will be presented.

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Session Classi ication: Poster Session 2

Contribution ID: **97** Type: **Poster**

Acoustic detection of intense GeV ion pulses

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Modern particle accelerators like the new SIS-100 synchrotron at the FAIR facility will deliver heavy ion beams of increasingly high intensities. New particle detections are required because existing detectors tend to saturate under these extreme conditions. This contribution presents an ionoacoustic detector, where the ion pulses are stopped in a water reservoir and the thermo-acoustic wave emitted at the point of maximum energy loss is detected by an ultrasonic transducer. In recent beamtimes at the SIS-18 of GSI, the detector was benchmarked under the irradiation with Xe, Pb and U ions of energies between 200 MeV/u and 1 GeV/u. The detector shows a linear response as a function of ions per pulse and by intensity variation, a large dynamic range was identified. Ion ranges measured with this technique are within 1% in agreement with ATIMA simulation and confirm ionoacoustics as a simple and accurate detection method for heavy ion beams.

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Presenter: KIRSCH, Leon

Session Classi ication: Poster Session 2

Contribution ID: **98** Type: **Poster**

Optimization of a target with a microchannel cooling structure using particle transport simulations

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The High Brilliance Neutron Source (HBS) project aims at developing a compact accelerator-driven neutron source (CANS) to deliver high brilliant neutron beams to a variety of neutron scattering instruments. For this, a compact tantalum target with a sophisticated internally microchannel cooling was developed for a 70 MeV proton beam with a peak current of 100 mA and an average power of 100 kW. The microchannel structure is optimized such that the neutron yield is increased and the protons will leave the target with a more uniform energy distribution, which minimizes the risk of blistering and produces a more homogenous energy deposition inside the target in order to minimize mechanical stresses. To get such an optimal design, simulations of different microchannel geometries were performed with Monte-Carlo simulation code FLUKA. The details of these investigations and the resulting microchannel target design will be presented.

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Session Classification: Poster Session 2

Contribution ID: **99** Type: **Poster**

Motion compensation in particle radiotherapy

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Cancers of moving organs as the lung have a poor prognosis with limited tumor control by conventional radiotherapy with photons. Particle therapy could improve patient outcome, but is challenged by non-periodic organ motion causing target miss and changes of the penetration depth of the ion beam.
We develop motion mitigation strategies for ion beam therapy, both in treatment planning software and dose delivery systems (DDS). We recently implemented 4D-optimization to the DDS of the clinical ion beam center CNAO, Pavia, Italy. The aim is to achieve conformal therapy that is robust against uncertainties in patient motion and anatomy. The figure shows the outcome of experiments at CNAO, comparing uncompensated and compensated dose delivery to the depicted motion trace.
In collaboration with CNAO, we will translate conformal particle therapy to clinical application, potentially offering treatment options to patients with currently low survival rates.

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Presenter: STEINSBERGER, Timo

Session Classification: Poster Session 2

Contribution ID: **100** Type: **Poster**

Morphological properties of polymer colloids on porous CNF layer

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Colloidal layer formation on porous materials is very relevant for functional coatings and printing. Our goal is to distinguish and quantify the topographical and the morphological layer formation of the colloidal layers during the deposition and annealing process between porous and solid templates above their glass transition temperature. Therefore, we compare cellulose nanofibers layer (CNF) as porous and silicon wafer as solid template. For the colloidal layers we use inks of poly(butyl methacrylate) and poly(sobrerol methacrylate) in aqueous dispersion.
To study the morphological layer formation during the deposition and annealing process of colloidal layers in real-time we used grazing incidence small angle X-ray scattering (GISAXS). During the deposition, the colloids partially enter the CNF layer and fill the CNF voids or remain on the CNF surface, leading to complex drying processes. The morphological of the CNF and colloidal layer changes when the glass transition temperature of the colloids is exceeded.

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Session Classification: Poster Session 2

Contribution ID: **101** Type: **Poster**

Femtomagnetism on the Nanoscale

Tuesday, November 23, 2021 1:30 PM (1h 40m)

We report on all-optically induced ultrafast magnetization dynamics in nanoscopic magnetic multi-domain states of Co/Pt multilayers employing time-resolved magnetic small-angle X-ray scattering (tr-mSAXS) at free-electron laser (FEL) facilities. We demonstrate the feasibility of optical-pump FEL-probe experiments on particularly thin Co/Pt multilayers with total film thicknesses of $d \leq 15\,\mathrm{nm}$ which are promising candidates for future all-optical switching (AOS) applications. From studying the ultrafast magnetization dynamics in dependence on the absorbed pump-pulse energy we propose that the critical slowing down of the remagnetization dynamics observed at high temperatures stems from the divergence of the spin specific heat at $T \approx T_{\mathrm{C}}$. In this high-temperature regime, we moreover find AOS-like permanent modifications on nanoscopic length scales that evolve independently from the ultrafast magnetization dynamics. A detailed analysis of both multi and single-shot measurements points at a novel AOS mechanism that involves the interplay between two light pulses of different photon energy.

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Session Classi ication: Poster Session 2

Contribution ID: **102** Type: **Poster**

Diamond formation kinetics in shock-compressed C-H-O samples via small angle X-ray scattering and X-ray diffraction

Tuesday, November 23, 2021 1:30 PM (1h 40m)

We present results for nanodiamond formation kenetics from C-H-O samples that were shock compressed to planetary relevant states via in situ X-ray diffraction and small angle X-ray scattering on LCLS and SACLA free electron X-ray laser (XFEL) facilities. The growing process of nanodiamonds during the shock compression history was observed unprecedentedly by two SAXS analysis methods. Diamond formation observed in three different C-H-O samples illustrates that this formation is mainly dependent on P-T conditions as well as initial stoichiometry in different samples. Density functional theory molecular dynamics simulations have well validated the pressure-temperature states at shock compressed conditions, greatly predicting the peak structure of the residual liquid mixtures to explain the demixing process in compressed C-H-O samples. The consistency of the experimental results on different XFEL facilities highlights a powerful potential of the new generation XFELs combined with in situ X-ray techniques in nanostructure detection related to planetary relevant science.

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Session Classification: Poster Session 2

Contribution ID: **103** Type: **Poster**

Towards new cutting-edge magnetorotational instability experiments – theoretical predictions

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Magnetorotational instability (MRI) is of paramount importance in astrophysics. It drives turbulence and angular momentum transport in accretion disks. Since 1990s, MRI has been extensively studied theoretically, first in its standard form (SMRI) with an axial magnetic field and later in its helical (HMRI) and azimuthal (AMRI) variants. Experimental confirmation of SMRI remains elusive, despite successful detections of HMRI and AMRI. The challenge lies in the extremely small magnetic Prandtl numbers of liquid metals, leading to high Reynolds numbers to trigger SMRI. The upcoming MRI experiment in frame of the DRESDYN project aims at attaining the high Reynolds and Lundquist numbers required for MRI. We present theoretical results for typical parameters of this experiment, which form the basis for ascertain MRI and interpreting the experimental outcomes. Another line of research is the application of Super-HMRI, which we discovered in rotating flows with positive shear, to the solar tachocline.

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Session Classification: Poster Session 2

Contribution ID: **104** Type: **Poster**

Dynamic structural studies of spike and antibody-spike complexes by combining SAXS and heterogeneous cryo-EM analysis

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the causative agent of the ongoing COVID-19 pandemic, is externally coated by a corona of spike proteins that bind to host cell receptors and trigger viral entry. The COVID-19 research and development landscape has developed rapidly over the last 2 years, where cryo-electron microscopy (cryo-EM) single-particle analysis has played a critical role in structurally characterising the spike protein. Single-particle cryo-EM has yielded the stable-state reconstruction(s) of the spike protein, but struggles to access information relating to the structural heterogeneity or intrinsic flexibility of the protein in solution. Here we combine heterogeneous cryo-EM analysis with small-angle X-ray scattering (SAXS) to probe the structural state(s) of the spike protein in solution that will broaden our understanding of the 'spike structural landscape' and provide a more complete picture of spike-neutralizing antibody and synthetic nanobody complexes targeted at therapeutically combatting the virus.

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Session Classi ication: Poster Session 2

Contribution ID: **105** Type: **Poster**

Pixel-wise crystal-diffraction moelling

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The recent diversification in macromolecular crystallographic experiments to pink beams, convergent electron diffraction and serial crystallography has shown the limitations of using the Laue equations for diffraction prediction. This publication aims to give a straightforward way of calculating approximate crystal diffraction patterns given varying distributions of the incoming beam, crystal shapes and other potentially hidden parameters. This enables modelling each pixel of a diffraction pattern, it improves the data processing of integrated peak intensities, by correcting the partially recorded reflections, and enable data processing, where it had not been possible before. The fundamental idea is to express the distributions as a weighted sum of Gaussian functions.

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Session Classification: Poster Session 2

Contribution ID: **106** Type: **Poster**

AXSIS X-band compact RF gun using pin cathode for photoemission

Tuesday, November 23, 2021 1:30 PM (1h 40m)

We discuss the design and first experimental tests of a compact X-band RF gun with a at 2.998 GHz, which can accelerate electrons up to 150 keV powered by only 10 kW of RF. A pin-cathode is used in the cavity to increase the RF electric field on the cathode up to 100 MV/m as in large-scale S-band guns. A solenoid is following the gun to focus the electron beam and achieve a transverse emittance of 0.1 mm mrad for up to 100 fC bunch charge. The experimental results show that there is good agreement with the designs and simulations. With the continuation of the conditioning, the electron multipacting (generation of electrons on surfaces exposed to an oscillating electromagnetic field) is gradually suppressed. Simulations show that the multipacting should disappear when applying to the cavity in addition a DC field resulting in an innovative very compact RF gun concept.

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Session Classification: Poster Session 2

Contribution ID: **107** Type: **Poster**

Effects of gate dielectric and ex-situ doping on electrical properties of transition metal dichalcogenide monolayer

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The precise control of dopant concentration and distribution in two-dimensional (2D) materials, e.g. transition metal dichalcogenides (TMDs), is a major problem on the way to their successful application in modern nanoelectronics. The use of capping layers is beneficial for a better doping control during ion implantation. In the present work, both optical and electrical properties of mechanically exfoliated 2D-TMDs with Al2O3, Si3N4 or SiO2 as gate dielectric layers have been explored. Using photoluminescence (PL) and Raman spectroscopies and current-voltage (I-V) characteristics we show that Al2O3 grown on monolayer TMDs by atomic layer deposition (ALD) shows the best device performance, while Si3N4 and SiO2 deposited by plasma enhanced chemical vapor deposition (PECVD) causes strong n-type doping. Moreover, the Cl+ ion implantation is successfully used to provide controlled doping of TMDs for a lateral p-n junction. This work shows new insights into controllable doping in 2D materials using ion implantation.

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Session Classification: Poster Session 2

Contribution ID: **108** Type: **Poster**

Heterogeneous catalytic ozonation and peroxone-mediated removal of Acetaminophen using natural and modified hematite-rich soil, as efficient and environmentally friendly catalysts

Tuesday, November 23, 2021 1:30 PM (1h 40m)

In the last decade, one of the most important issues considered by Environmental Engineers was related to water pollution. Catalytic ozonation was developed as a promising method for removal of acetaminophen due to its high activity and strong oxidation ability. In this study, Red Soil (RS), was used as an environmentally friendly catalyst in the catalytic ozonation of acetaminophen before its discharge into the environment. After calcination (C), C-RS nanoparticles exhibited high activity in degradation of acetaminophen combined with O3 and H2O2/O3. The high activity of C-RS was related to the structural modification of RS during the calcination process and the formation of oxygen vacancies as active catalytic sites. In peroxone process, the formation of the Fe3+/Fe2+ cycle and the synergy effects between O3 and H2O2 results in the formation of HO•. This natural catalyst can be used as precursor for the fabrication of hematite-based nanocomposites for advanced oxidation processes.

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Session Classification: Poster Session 2

Contribution ID: **109** Type: **Poster**

The Advanced XAFS-Beamline P64 at PETRA III/DESY

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The beamline P64 at the electron storage ring PETRA III at DESY is dedicated to x-ray absorption fine structure (XAFS) measurements with application in many scientific disciplines. XAFS is an element specific technique which probes the local environment of the absorbing element and determines its nominal valence. Conventional XAFS-measurements are performed in transmission or fluorescence geometry on the minute timescale. At P64, we have several advanced techniques: By **oscillating** the **monochromator** with frequencies between 0.5 and 50 Hz, we can measure 1-100 XAFS-spectra within 1s, which helps to understand chemical reactions under changing conditions. A **high-resolution emission spectrometer** helps to overcome the lifetime broadening of the absorption edge in order to observe transitions in the pre-edge region with better energy resolution. The emission is measured with high energy-resolution in order to gain complementary information. Recently, we added a **laser** for pump probe spectroscopy for investigations of the exited state.

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Session Classification: Poster Session 2

Contribution ID: **110** Type: **Poster**

In-situ AFM nanomechanical mapping of ultrathin polypyrrole films in a liquid electrolyte as a function of the electrical potential

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Polypyrrole is a conductive polymer and well known for showing volume changes when applying an electrical potential in an electrolytic medium. Its potential use as actuator, sensor, capacitor, and many more has been the driving factor for a large volume of work done in this field. However, for applications it is essential to understand the processes and mechanical forces a polypyrrole film exerts during electrochemical cycling. We present an in situ microscopic study of the actuation and elastic modulus of an ultrathin (<100 nm), silicon substrate-supported polypyrrole film under electrochemical conditions. The film thickness increases upon oxidation and decreases during reduction, an effect caused by the anion and proton transfer into and out of the film. The Young's modulus of the film changes in conjunction with the height and potential, and the surface shows modulus variations that we assign to the typical cauliflower-like surface topography.

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Presenter: Mr MEINHARDT, Alexander (DESY)

Session Classification: Poster Session 2

Contribution ID: **111** Type: **Poster**

Structural dynamics and shape changes of supported palladium nanoparticles

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Understanding the dynamics, such as structural and shape changes observed in oxidation and reduction reactions of metal nanoparticles are crucial for understanding of fundamental processes in heterogeneous catalysis. These processes occur at high temperatures and under gas exposure on time scales of femtoseconds to nanoseconds. The aim of this work is to investigate these dynamics of Pd nanoparticles supported on MgO(001) in chemical reactions and in a pump-probe manner. It has been shown that, 14 nm sized Pd nanoparticles with change shape upon oxygen exposure and their behaviour is dependent on their initial orientation, size and shape. Lab based and European XFEL time resolved X-ray diffraction experiments have elucidated transient laser heating processes on the femto- and nano- second time scale. These experiments provide a basis for future experiments utilising lasers to trigger reactions investigating nanoparticle shape changes in catalytic conditions.

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Session Classification: Poster Session 2

Contribution ID: **112** Type: **Poster**

Dimensional crossover in NbSe3 under Extreme Conditions

Tuesday, November 23, 2021 1:30 PM (1h 40m)

High pressure and low temperature single crystal XRD, electronic and magnetic transport measurements on NbSe3 are performed and found that a dimensional crossover maybe happened at 0.8 GPa, accompanied with a positive to negative MR evolution and p-n Hall resistivity anomaly. Most important is q2 vector = (0.5, 0.263, 0.5), which exists mainly on the Nb atoms of type I, disappeared at the same pressure suggesting absent of a novel 1D order and fully developing its higher-dimensional coherence under extremely condition. With further increasing pressure, the ambient pressure q1 vector = (0, 0.243, 0) changed to (0, 0.233, 0) at 2.5 GPa, then quenched with the superconductor emerged at 3.6 GPa. Our study on NbSe3 will help to systematize the broader class of q1D metallic system, the similarities and differences of their properties and the limits of the FS adjustment by compression.

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Session Classification: Poster Session 2

Contribution ID: **113** Type: **Poster**

Studying vacuum conditions for vacuum birefringence experiments

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Exploring vacuum birefringence by combining high intensity PW-class optical lasers with X-ray free electron lasers (XFEL) is a very attractive research field. Due to the tiny signal of vacuum birefringence, it is prerequisite to eliminate the influence of charged particles generated from the residual gas by the ionization with the PW laser. This can be done by a static electric field and a preceding laser pulse: Charged particles will be generated but removed prior to the XFEL pulse arrival. For appropriate conditions of the ionized volume and static field strength, a short 'vacuum' time is available when electrons and ions are swept out of the interaction volume and residual gas particles are not yet back by thermal motion.
We present studies of that scheme with a downscaled double-pulse setup and a time of flight (TOF) ion detection.

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Session Classification: Poster Session 2

Contribution ID: **114** Type: **Poster**

Ptychography at FELs: diffraction-limited and time-resolved imaging of extended samples.

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Free electron lasers (FELs) emit ultra-bright, femtosecond-long and highly coherent pulses which makes them ideal for high-resolution imaging. Therefore, they became tool of a choice for coherent diffraction imaging techniques. However, most of these techniques are developed for the imaging of nano-samples and not applicable for extended objects. At the same time, ptychography, a scanning X-ray imaging method, found a wide area of applications at synchrotrons. It allows imaging of extended samples with diffraction-limited resolution, but is hard to implement at FELs due to spatial fluctuations of photon beams.
We present our adaptive automatic differentiation powered implementation of ptychography, which is capable of working with partially coherent and spatially fluctuating pulses of FELs and allowed us to perform multiple successful imaging experiments. Additionally, we present a single-shot extension of this method capable of performing time-resolved imaging of extended objects and the first results obtained.

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Session Classification: Poster Session 2

Contribution ID: **116** Type: **Poster**

Study of chemical bonds in metal-oxygen systems based on X-ray absorption spectroscopy

Tuesday, November 23, 2021 1:30 PM (1h 40m)

To understand chemical bonds between transition metals and oxygen is of great scientific and technological interests in view of different types of oxo-ligands and unusual oxidation states, and their dependence on electronic structure and stoichiometry. Here, we use X-ray absorption spectroscopy (XAS) at the metal $L_{2,3}$ or $M_{2,3}$ and oxygen K edges of $[MO_n]^+$ systems (M = transition metal, n = integer) to correlate the spectroscopic signatures with the type of oxo-ligand (oxo, peroxo, superoxo or oxyl) and correctly assign the oxidation state of the metal center. XAS experiments are performed on size selected $[MO_n]^+$ species in the gas phase, produced by a magnetron sputter source. The cationic species are mass selected using a quadrupole mass filter and investigated in a cryogenic ion trap. Our ion trap instrument is installed at the undulator beamline UE52-PGM at the Berlin synchrotron radiation facility BESSY II.

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Session Classification: Poster Session 2

Contribution ID: **117** Type: **Poster**

3D Active Sites of Te in Hyperdoped Si by Hard X-ray Photoelectron Kikuchi-Diffraction

Tuesday, November 23, 2021 1:30 PM (1h 40m)

n-type doping of Si by the deep chalcogen donor Te in excess of the solubility limit was recently demonstrated to lead to hyperdoped material [1]. Our investigation by hard x-ray photoelectron spectroscopy (hXPS) reveals at least two different Te species with different binding energy and systematically varying concentrations with increasing ion implantation dose. At the highest doping we study the photoelectron scattering patterns using hard x-ray photoelectron diffraction (hXPD). Substitutional site occupation of both Te monomers as well as dimers is identified with increasing binding energy leading to the main features in the XPS spectra. The sharp hXPD patterns allow the detailed analysis of the local surrounding of the dopant atoms. At the lowest binding energy an additional species is found and the distinct, rather diffuse hXPD pattern at this binding energy suggests the assignment of this component to a small fraction of Te in clusters.

[1] M.Wang etal. Phys.Rev.Appl.*11_054039*(2019)

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Session Classification: Poster Session 2

Contribution ID: **118** Type: **Poster**

Selene guides for macromolecular diffractometers

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Typical samples in protein crystallography have a size well below 1 mm. At the same time, a fairly narrow collimation is required to provide sufficient momentum transfer resolution. While these requirements are easily fulfilled by synchrotron beams, neutron beams are typically much larger and tailored to the sample size in the vicinity of the sample. The concept of SELENE neutron optics enables the beam spot shaping at a virtual source position far away from the sample [1]. Here we present the optimization for a macromolecular diffractometer at a HIgh Current Accelerator driven Neutron Source (HICANS). Our results show very efficient imaging of the virtual source onto the sample position with gapless divergence and phase-space distributions, which is also insensitive to gravity effects. This work is the first important step towards the design of the single crystal diffractometers for the Jülich High Brilliance neutron Source (HBS)[2].

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Session Classification: Poster Session 2

Contribution ID: **119** Type: **Poster**

Anomalous Hall effect and magnetic structure of the topological semimetal - Hexagonal-(Mn0.78Fe0.22)3Ge

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The location of the Weyl nodes can be tuned by suitable dopants of the Mn3Ge, such as Fe on the Mn site. Therefore, to demonstrate control over the topological Weyl nodes, we have grown single crystals of (Mn0.78Fe0.22)3Ge, and studied the magneto-transport properties and magnetic order with neutron diffraction. We find that (i) the chiral anomaly and AHE were a magnitude smaller than that in Mn3Ge and (ii) that the 22%Fe-doped sample also possesses Mn3Ge type magnetic structure in the temperature regime where AHE was observed. Our results demonstrate that the location of Weyl points and their separation can be tuned significantly by suitable dopants of the Weyl semimetals, which can eventually lead to control of the AHE observed in the sample.

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Session Classi ication: Poster Session 2

Contribution ID: **120** Type: **Poster**

Conveyor belt-based sample delivery system for multi-dimensional serial crystallography

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Serial crystallography at both X-ray Free-electron Lasers (XFELs) and synchrotrons offers the possibility to collect data at room temperature almost radiation damage free and enables time-resolved crystallography. The necessary steady delivery of new micron-sized crystals of biological macromolecules sets it apart from traditional single crystal macromolecular crystallography (MX). For this, many new means of sample delivery have been developed. Described here is a novel conveyor belt-based sample delivery system, the completely re-designed and re-engineered second generation of the CFEL TapeDrive. It is optimized for fast installation at beamlines, ease of use and precise adjustment of several sample delivery parameters, including a novel approach for sample temperature control. These developments enable fast SSX data collection – approaching the 10-seconds-per-dataset-limit – as well as successful structure determination of three different proteins at temperatures up to 317 K. Thus, CFEL TapeDrive2 is paving the way towards multi-dimensional serial crystallography.

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Session Classi ication: Poster Session 2

Contribution ID: **121** Type: **Poster**

Sunny Cellulose

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Cellulose nanofibrils (CNF) as a bio-based resource-saving and renewable material are very attractive due to their biocompatibility, flexible, lightweight, transparent and good mechanical strength. In this project we are going for building-integrated photovoltaics. In detail, we develop a combination of the CNF and sprayed-on solar cells. Solar cells with PEDOT:PSS as electron blocking layer, P3HT:PCBM as photoactive layer and ZnO as hole blocking layer will be designed both in standard and inverted devices. Ag nanowires can be used as electrode material. Spray deposition will be used as a suitable technique to fabricate such functional layers in a large scale with homogeneous surface and a low roughness.
To optimize the process through the formation of nanostructure during spraying and to obtain a higher efficiency of solar cell, in-situ grazing incidence small- and wide-angle X-ray scattering (GISAXS/GIWAXS) will be used to observe the nanostructuring of each layer material.

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Presenter: Dr CHEN, Zimei (DESY)

Session Classification: Poster Session 2

Contribution ID: **124** Type: **Poster**

The mechanism of few-layer graphene growth on silicon carbide substrate

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The study of the UHV synthesis of few-layer graphene on cubic SiC(001) substrate was performed using ARPES, LEEM, and μ-LEED. The thickness of the graphitic overlayer supported on the silicon carbide substrate and related changes in the surface structure are accurately controlled by observing the evolution of the surface graphitization in situ during high-temperature graphene synthesis. The graphitization of the cubic-SiC(001) surface starts from the formation of nanodomains with their graphene lattices aligned relative to the silicon carbide crystal lattice. The growth of such nonrotated graphene domains is favored by the small mismatch between the c(2×2) and graphene lattices. At sub-monolayer coverages, these nonrotated graphene domains dominate, with the nonrotated and rotated domains coexisting in the first completed monolayer. The gradual changes in the preferential graphene lattice orientations during further the few-layer graphene growth on SiC(001) were observed. The data can be used for the controllable growth of few-layer graphene

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Presenter: Prof. ARISTOV, Victor (DESY)

Session Classification: Poster Session 2

Contribution ID: **127** Type: **Poster**

Multi-phase In nanoparticles formation in CuPcF4 studied by TEM and PES in UHV

Tuesday, November 23, 2021 1:30 PM (1h 40m)

We present the investigation of the morphology and electronic properties of the nanocomposite material consisting of the thin CuPcF4 film and multiphase/multidimensional indium nanoparticles, self-organized on the surface and in the bulk of the organic matrix during synthesis in UHV. The HR-TEM pictures delivered information about the development of morphology, size, density, and distribution of In nanoparticles upon indium deposition. These 2D/3D ultra-small indium nano-objects turned out to have not only body-centered tetragonal (bct) crystal structure, typical for bulk indium, but also an unusual fcc one. The studies of the electronic structure of the hybrid nanocomposite on variable stages of metal deposition were performed by XPS and NEXAFS. We have found weak interaction of indium with CuPcF4, while valence band spectra have shown an essential evolution of the electronic properties of the compound. The results can be applied for the creation of new prototypes of metal-organic memory devices.

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Session Classification: Poster Session 2

Contribution ID: **128** Type: **Poster**

Ionic liquids in mild nanoscopic confinement

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The structure and dynamics of the ionic liquid 1-ethyl-3-methylimidazolium acetate (EMIMAc) in porous glass with pores of the size 40 and 100 Å is determined in comparison to the bulk liquid. We employed x-ray diffraction to measure the domain structure, and neutron backscattering for the dynamics. In confinement, the liquid displays onion-like domain structuring while in bulk the liquid is largely forming a bicontinuous structure similar to microemulsions. This also has an effect on the dynamics of the liquid at high temperatures (373K): The ions in the bulk can diffuse along the domain boundaries while they need to cross the domains in the ordered state in confinement. At low temperatures, the attractive forces of all ions are such strong that the diffusion in any direction is similarly slow, and the exact domain structure is less important.
[1] D. Noferini, O. Holderer, H. Frielinghaus, Physical Chemistry Chemical Physics, 22, 9046 (2020).

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Session Classification: Poster Session 2

Contribution ID: **129** Type: **Poster**

Recovery of nanodiamond produced in laser induced shockcompression

Tuesday, November 23, 2021 1:30 PM (1h 40m)

The extreme pressure and temperature conditions in the icy giants, Neptune and Uranus, can be reproduced using laser-driven shock compression. When reproducing these conditions in the laboratory the formation of nanodiamonds (ND) was observed in polystyrene and PET.

The formation process of the NDs itself is not yet completely understood. It is suggested that the possible insulator-metal transition of hydrogen expected in this regime may play a key role. NDs have many applications and their intact recovery could open the way for a new laser compression synthesis path. Since the NDs are ejected at hyper-velocities and as part of a debris cloud, their intact recovery is a challenging task.

Most recent data from a recovery campaign in September this year will be presented. The data obtained might open the path towards dynamic material synthesis generally and deepen the understanding of the phase separation process at planetary interior conditions.

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Session Classification: Poster Session 2

Contribution ID: **130** Type: **Poster**

Adsorption of Organic Acids on Magnetite Surfaces

Tuesday, November 23, 2021 1:30 PM (1h 40m)

Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications as a catalyst in various industrial processes such as the water-gas shift reaction. In material science magnetite nanoparticles are linked by oleic acid to form supercrystals with exceptional mechanical properties. However, only little is known about the interaction at the oxide/organic acid interface. In this contribution the adsorption of formic acid (HCOOH) and oleic acid ($C_{17}H_{33}COOH$) on the magnetite (111) and (001) single crystal facets is studied under UHV conditions at room temperature. Our experimental results and theoretical calculations provide insight into molecule adsorption geometries and layer properties as well as near-surface structural changes in magnetite after molecule adsorption. The experiments were performed at the DESY NanoLab, Centre for X-ray and Nano Science, and the ID03 (ESRF) and SIXS (Soleil Synchrotron) beamlines.

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Session Classification: Poster Session 2

Contribution ID: **144** Type: **Poster**

Towards imaging X-ray polarimetry as community setup at HED

Wednesday, November 24, 2021 1:30 PM (1h 40m)

X-ray polarimetry is an attractive technique which opens the route to study polarization effects with X-rays. Faraday rotation is widely know in plasma physics to study magnetic field structures. With the extension towards X-ray wavelengths, solid density plasmas can be probed, what is in particular interesting for plasmas driven by ultra-intense lasers.
We are developing a standard setup for the community to study magnetic fields in laser-driven solid density plasma samples or further effects being detectable by polarimetry with limited purity. This development is equally important for studying strong-field QED phenomena like vacuum birefringence at XFELs since it investigates and compares various technological approaches as well as experimental techniques and practices.

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Session Classi ication: Poster Session 2

Contribution ID: **167** Type: **Poster**

Site-selective cation transport in the near-surface region of magnetite

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The structure and stoichiometry in the near-surface region of magnetite (Fe_3O_4) critically influencing the performance of magnetite-based catalysts and devices are altered by cation transport processes at elevated temperatures [1]. Nuclear forward scattering (NFS) was used to track the ^{57}Fe transport at the interface of a homoepitaxially grown $^{57}Fe_3O_4$ layer and a (001) oriented Fe_3O_4 substrate during stepwise ultra-high vacuum annealing. A simultaneous fit of nuclear resonant reflectivities and timespectra [2] measured after each step generated site selective ^{57}Fe-depth profiles indicating a notable site-dependence of the near-surface cation transport between 470-710 K and reduced diffusion coefficients compared to the bulk. The structural characterisation of similar thin-films by surface X-ray diffraction confirmed a slight cation deficit in the thin-films also suggested by NFS that maybe influenced the transport process.
[1] Arndt et al. Chem. Comm. 1, 92 (2019) [2] Andreeva et al., Mosc. Univ. Phys. Bull. 63, 132 (2008)

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Session Classi ication: Poster Session 2

Contribution ID: **165** Type: **Invited Talk**

Physics of the Sun

Tuesday, November 23, 2021 3:10 PM (20 minutes)

The Sun’s energy is generated by stellar hydrogen burning in proton-proton (pp) chains. The solar neutrino producing pp-II and pp-III chains start with the reaction ³He(α,γ)⁷Be. At higher temperatures, the same reaction is responsible for ⁷Li production in Big Bang Nucleosynthesis (BBN). At the underground accelerator laboratory Dresden Felsenkeller, a comprehensive study of this reaction via in-beam γ-spectroscopy and activation is under way. Further, new and precise cross-section measurements of BBN deuterium burning will be presented that are in excellent agreement with a recent analysis of the cosmic microwave background (CMB). Complementary efforts at the radiation source HZDR ELBE and other facilities will be discussed,
as well.

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Session Classification: Session F

Contribution ID: **122** Type: **Invited Talk**

Dielectronic Recombination Spectroscopy at CRYRING@ESR

Tuesday, November 23, 2021 3:30 PM (20 minutes)

During the GSI beamtime campaign in spring 2021 the first merged-beam DR measurements were performed at the CRYRING@ESR electron cooler since its move from Stockholm. For this purpose a new particle detection and data acquisition setup were installed and tested in 2020. Taking advantage of the access to the GSI accelerator chain, DR of Pb^{78+} was measured in March as a test run for future atomic physics experiments on highly-charged ions. This experiment was followed in May by measurements on Ne^{2+} and O^{6+} which were injected from a local ECR source. The neon experiment focused on obtaining absolute rate coefficients for low-energy transitions that are needed for accurate modelling of astrophysical plasmas. The goal of the oxygen experiment was the observation of trielectronic recombination (TR).
This contribution will present details about our new measurement setup and the experiments performed, with a particular focus on the results of the neon measurement.

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Session Classification: Session F

Contribution ID: **24** Type: **Invited Talk**

Element-selective x-ray spectroscopy under pulsed high magnetic fields

Tuesday, November 23, 2021 3:50 PM (20 minutes)

Strong magnetic fields are used to study various electronic and magnetic properties of materials as a tunable external parameter that controls and modifies the state of matter. Non-destructive magnetic fields up to 100 T are available in state-of-the-art high-field facilities. However, in other large-scale facilities such as synchrotrons and x-ray free-electron lasers, the application of such high magnetic fields has been limited due to various restrictions. In this talk, I will present our recent studies using element-selective soft x-ray magnetic circular dichroism measurements under pulsed high magnetic fields. This enables us to study microscopic magnetic properties of magnetic-field-induced phases, which is challenging to obtain directly from conventional macroscopic measurements, especially for magnetic materials composed of more than two magnetic ions. I will discuss the nature of field-induced phases in the magnetic frustrated system MnCr2S4 and 3d-4f intermetallic compounds in high magnetic fields.

Primary author: YAMAMOTO, Shingo

Presenter: YAMAMOTO, Shingo

Session Classification: Session F

Contribution ID: **125** Type: **Invited Talk**

Examples of Restricted Subspace Approximated TD-DFT Calculations for on-the-fly Analysis of Experimental X-ray Spectra

Tuesday, November 23, 2021 4:10 PM (20 minutes)

In this contribution, we discuss a protocol for calculating resonant inelastic X-ray scattering (RIXS) cross-sections applying the restricted subspace approximation (RSA) to time-dependent density functional theory. Specifically, the necessary core and valence occupied orbitals are included in the donor space, while the virtual acceptor space is truncated, allowing for the efficient evaluation of both the core- and valence-excited state manifolds within a single TD-DFT calculation. The method can be run in a nearly black-box fashion, enabling quick prediction and evaluation of experimental RIXS spectra by non-expert users. The low computational cost also allows for the investigation of large molecular systems and explicit solvation effects. Recent examples from RIXS experiments in solution phase carried out at the BESSY II synchrotron will be presented.

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Session Classification: Session F

Contribution ID: **193** Type: **Invited Talk**

Depth-resolved phase and residual stress analysis with white hard X-rays at the new beamline P61A

Tuesday, November 23, 2021 4:30 PM (20 minutes)

Presenter: ABREU FARIA, Guilherme (HZ Hereon)

Session Classification: Session F

Contribution ID: **12** Type: **Invited Talk**

Polymer dynamics in nanocomposites studied by neutron scattering.

Wednesday, November 24, 2021 9:00 AM (20 minutes)

Grafting polymer chains on nanoparticles prevents their undesired aggregation finally leading to improved properties. It is particularly important for solvent-free nanocomposites consisting of grafted nanoparticles. Dynamics of grafted chains is different from that of free polymer. As a result, macroscopic properties, e.g. viscoelasticity, are influenced. Recent reports lack consensus on whether the local dynamics of grafted chains is accelerated or retarded. We study segmental dynamics of polyisoprene grafted on spherical nanoparticles using neutron backscattering. The analysis of relaxation times led to the following conclusions: (i) Low molecular weight (MW) OCNC display reduced local relaxation (ii) At high MW and equal grafting density faster segmental dynamics than the free polymer is observed. We prove that these conflicting results are seemingly artifacts of the traditional analysis. We invoke an elegant methodology and show that the underlying physics of grafted polymer is unchanged. However, its spatial variation causes the average dynamics to transition.

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Presenter: SHARMA, Aakash (JCNS-1, Forschungszentrum Jülich)

Session Classification: Session G

Contribution ID: **35** Type: **Invited Talk**

Cu nanowire networks as catalyst for electrochemical CO2 reduction

Wednesday, November 24, 2021 9:20 AM (20 minutes)

Three-dimensional interconnected copper nanowire networks are synthesized by ion-track nanotechnology and electrochemical deposition. By sequential swift heavy ion irradiation of polymer foils from four different directions, interconnected ion-tracks are generated. The ion-tracks are selectively dissolved and enlarged to form an interconnected nanochannel network, in which the copper nanowires are electrodeposited. Subsequent dissolution of the polymer leads to free-standing nanowire networks with electrochemically active surface areas of up to 500 cm2 on a geometrical sample area of just 1.77 cm^2. The Cu nanowire networks are applied as catalyst for electrochemical CO2 reduction. The conversion efficiency towards liquid and gas phase products is studied as a function of applied potential. Morphology and crystalline structure of the nanowire networks are investigated before and after CO2 reduction by scanning electron microscopy and X-ray diffraction, respectively, evidencing that the structure of the network remains stable with no changes in surface area and structure.

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Presenter: ULRICH, Nils Max (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI))

Session Classification: Session G

Contribution ID: **70** Type: **Invited Talk**

Transport properties of tailored semimetal bismuth nanowires synthesized by ion-track nanotechnology

Wednesday, November 24, 2021 9:40 AM (20 minutes)

Due to the large Fermi wavelength and mean free path of charge carriers in bismuth, Bi nanowires with tailored geometry are excellent model systems to investigate quantum and mesoscopic transport properties. Additionally, these unique properties make them promising candidates for various applications such as e.g. infrared sensor.
The combination of ion-track nanotechnology and electrodeposition provides an excellent platform to fabricate tailored nanowires for the investigation of size-dependent properties. Etched ion-track membranes are fabricated by swift heavy ion irradiation and subsequent chemical etching of polymer foils. Symmetric and asymmetric etching conditions are applied to fabricate cylindrical and conical nanochannels, respectively. Subsequent electrodeposition in the channels results in arrays of bismuth nanowires with cylindrical or conical geometry, with diameters as small as 20 nm.
This talk presents an overview of our investigations of the Seebeck coefficient and electrical resistance of bismuth nanowire arrays as a function of geometry, nanowire diameter and temperature.

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Presenter: WAGNER, M.F.P. (GSI Helmholtz Center)

Session Classification: Session G

Contribution ID: **132** Type: **Invited Talk**

Lattice Dynamics of α-FeSi2 Nanostructures

Wednesday, November 24, 2021 10:00 AM (20 minutes)

Iron silicide is a particularly interesting member of the technologically important class of transition-metal silicides, since it is the only representative that forms metallic and semiconducting phases. In this talk, I will present recent results on the lattice dynamics of α-phase $FeSi_2$ nanoislands and nanowires, epitaxially grown on silicon surfaces. The phonon density of states (PDOS) of the nanostructures was experimentally obtained by nuclear inelastic scattering and additionally determined by *ab initio* calculations. The experimental results reveal a distinct anisotropy of the PDOS along and across the nanowires, which is not present in the nanoislands. These results can completely be understood under consideration of the specific orientation of the α-FeSi2 unit cell on the Si surface. Furthermore, both kinds of nanostructures show a distinct damping of the PDOS features upon reduction of the characteristic sizes, which can be comprehended by modeling of the experimental results with the *ab initio* calculations.

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Presenter: KALT, Jochen (Karlsruher Institut für Technologie)

Session Classification: Session G

Contribution ID: **57** Type: **Invited Talk**

Magnetization dynamics in curved magnetic membranes and three-dimensional nanostructures

Wednesday, November 24, 2021 10:20 AM (20 minutes)

Spin waves (magnons), the small-amplitude excitations of ferromagnets, are promising candidates for future computation applications, providing intrinsic nonlinear behavior, nonreciprocal wave propagation, and, among other things, a versatile interface to spin qubits. Over the last decades, countless works have investigated the dynamics and possible applications of spin waves in magnetic thin films, rectangular wave guides, multilayers and other flat structures. However, the physics of ferromagnets and their excitations change considerably when transitioning from quasi-2D to 3D structures. Curvature and 3D geometry have been shown to introduce effects which are not present in flat systems of the same material. For example, surface curvature can stabilize magnetic skyrmions, or lead to a dipolar-induced asymmetric spin-wave dispersion. In this talk, we will use micromagnetic simulations to explore the field of curvilinear spin-wave dynamics, which combines aspects of symmetry, topology and nonlinear physics.

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Presenter: KÖRBER, Lukas (Helmholtz-Zentrum Dresden - Rossendorf)

Session Classi ication: Session G

Contribution ID: **195** Type: **Invited Talk**

Current developments in the research field “Matter”

Wednesday, November 24, 2021 11:00 AM (20 minutes)

Presenter: DOSCH, Helmut

Session Classification: Session H

Contribution ID: **173** Type: **Invited Talk**

Hard X-ray photoelectron spectroscopy of Cu(In,Ga)Se2 thin-film solar cell interfaces

Wednesday, November 24, 2021 11:20 AM (20 minutes)

In this work, we have investigated the interface between a Cu(In,Ga)Se2 (CIGSe) absorber prepared with an in-line co-evaporation process and a sputter-deposited GaOx buffer layer. The chemical and electronic structure of this interface is crucial for device performance and was studied using hard x-ray photoelectron spectroscopy (HAXPES) at the X-SPEC beamline of the KIT synchrotron, as well as x-ray photoelectron spectroscopy (XPS) in the Materials for Energy (MFE) laboratory. X-SPEC is a high-flux undulator beamline with a photon energy range of 70-15000 eV, which allows a wide variation in electron kinetic energies, much beyond the range of laboratory-based methods.

With the combination of our spectroscopic techniques, a detailed and depth-varied picture of the chemical and electronic structure of the CIGSe surface and its interface with GaOx can be painted. The results are also discussed in view of the device performance, particularly focusing on surface treatments prior to GaOx sputter deposition.

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Session Classification: Session H

Contribution ID: **6** Type: **Invited Talk**

Charge Carrier Screening in Photoexcited Epitaxial Semiconductor Nanorods Revealed by Transient X-ray Absorption Linear Dichroism

Wednesday, November 24, 2021 11:40 AM (20 minutes)

Understanding the electronic structure and dynamics of semiconducting materials at the atomic level is crucial for the realization and optimization of devices in solar energy and photocatalysis. Unidimensional carrier transport in oriented nanorod arrays is a promising development for enhanced performances in solid-state solar cells. Epitaxial ZnO nanorods in particular have emerged as promising candidates due to the piezophototronic tunability of electronic conduction. Here, we report on the picosecond dynamics of atoms and charge carriers in photoexcited epitaxial ZnO nanorods by time-resolved X-ray absorption linear dichroism. The transient signal is composed of incoherent atomic thermal motion and non-local screening of the core-hole potential by photogenerated electron-hole pairs. In addition, we observe transient phase-space filling in the pre-edge. Our results open new perspectives for the study of charge carriers in photoexcited semiconductor materials from an atomic perspective, which should prove useful in materials and devices composed of multiple chemical elements.

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Session Classification: Session H

Contribution ID: **67** Type: **Invited Talk**

Structure-property relationships in caloric materials

Wednesday, November 24, 2021 12:00 PM (20 minutes)

Industrial refrigeration applications contribute a substantial part to mankind's energy consumption. New technologies based on solid-state caloric effects, such as magnetocaloric and barocaloric, promise considerable efficiency compared to today's vapor-compression technology. Within our research, we aim for a better understanding of the relation between the material structure and dynamics.

In this talk, we will discuss, how the structure and microscopic dynamic correlate with the caloric effects in the magnetocaloric compound family $Mn_{5-x}Fe_xSi_3$ [1,2] and in the spin-crossover material $Fe(Pm{-}Bia)_2(NCS)_2$, which exhibits a large barocaloric effect at modest hydrostatic pressure [3]. Our results on the two different polymorphs of $Fe(Pm{-}Bia)_2(NCS)_2$ compound show a different temperature evolution across the transition, indicating the importance of the crystalline structure.

[1] N. Biniskos, et al., Phys Rev B. 96, 104407, 2017.

[2] P. Hering, et al.,Chem. Mater. 27, 7128, 2015.

[3] K. G. Sandeman, APL Mater., vol. 4, no. 11, pp. 4–9, 2016.

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Session Classification: Session H

Contribution ID: **4** Type: **Invited Talk**

Self-assembly of Au-Fe3O4 dumbbell nanoparticles

Wednesday, November 24, 2021 12:20 PM (20 minutes)

Dumbbell nanoparticles (DBNPs) consist of optically active Au and magnetic iron oxide nanoparticles. Control and manipulation of these multifunctional heterostructures have applications in dual-probe biomedical imaging, catalysis, sensing, optics and electronics. Self-assembly of DBNPs of different sizes, coated with a mixture of oleic acid and oleylamine dispersed in a solvent, is investigated using small-angle x-ray and neutron scattering in an applied magnetic field. We compare the effects of complex morphology against its spherical counterparts: the single-phase iron oxide nanoparticles. Several parameters including size, distribution, the thickness of surfactant coating, composition, and magnetic structure, play a significant role in the formation of assemblies. Multiscale experiments and reverse Monte Carlo simulations provide a detailed parametric study to unravel the mechanisms of self-assembly in DBNPs.

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Session Classification: Session H

Contribution ID: **40** Type: **Invited Talk**

Structure function relationship in spider attachment hairs

Wednesday, November 24, 2021 12:40 PM (20 minutes)

The hairy attachment system of spiders enables these animals to walk upside-down on rough and smooth surfaces without the use of glue. These outstanding biological structures include hundreds to thousands of specially structured hairs. However, it is not completely understood how the structural features of the finest contact elements of single attachment hairs and their changes guide the attachment process.
The goal of our study is to gain an in-depth understanding of the working principle of the attachment and detachment processes of single hairs to the surface. Synchrotron-based methods like scanning X-ray nanobeam diffraction and high resolution X-ray nanotomography are ideal tools to reveal the inner structure of the spider hairs, especially the gradient of the mechanical properties, which is essential for the attachment process. A single attachment hair was attached and detached force-controlled from a surface in in situ experiments, which have been performed successfully with both methods.

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Session Classi ication: Session H

Contribution ID: **131** Type: **Poster**

Characterising Insulator-metal transition of Hydrogen with spectrally resolved X-ray scattering

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The giant planets have dominated the numbers in the ever-increasing list of exoplanets. Efforts to understand the internal structures of these giants have been going on for a few decades. There have been numerous experimental and theoretical endeavors, but there is still a long way to go for a proper understanding of the interiors. The insulator-metal transition in hydrogen is an important phenomenon to understand interiors of gas giants like Jupiter and Saturn and the physical and chemical behavior of highly compressed condensed matter. We discuss a potential approach to characterize the formation of metallic hydrogen in dynamically compressed plastic samples by spectrally resolved X-ray scattering. With the help of time-dependent density functional theory (TDDFT) calculations and data collected in a previous experiment at European X-ray Free-Electron Laser (EuXFEL), we give an outlook of future experiments and canvass the possibilities with the drive laser system at EuXFEL.

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Presenter: RANJAN, Divyanshu (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Poster Session 3

Contribution ID: **134** Type: **Poster**

Selection and control of (bio)nanoparticles with electric fields

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Single-particle imaging (SPI) experiments at free-electron lasers (FELs) promise high-resolution-imaging of the structure and dynamics of nanoparticles and macromolecules. Guiding sample particles into the focus of an FEL, diffraction patterns of individual particles can be collected. Sufficient amounts of patterns of identical nanoparticles are needed to overcome the inherently small signal-to-noise ratio and reconstruct the underlying 3D structure. Size-optimized delivery of identical nanoparticles is key to efficient and successful SPI experiments. Here, we present approaches for the production of purified high-density beams of a broad variety of biological nanoparticles. We establish control through electric fields, aiming at charge state or conformational state selectivity. This is especially relevant for soft biological samples, such as proteins or protein complexes, which in uncontrolled environment are prone to structural instability.

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Presenter: SAMANTA, Amit (CFEL-DESY)

Session Classification: Poster Session 3

Contribution ID: **135** Type: **Poster**

Integrated X-ray techniques for durable dental interzones

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Nowadays teeth are not directly extracted when tooth decay occurs. Whenever treatment is pos-sible, the carious region is replaced with a suitable filling with the filling material dependent on the position and size of the cavity. Since the restoration will remain in the tooth for many years, a well adhering and sealing interface between filling and healthy tooth tissue is needed. Intensive studies of this complex interface are still lacking. Little is known about possible diffusion of ele-ments from dental materials into healthy tooth tissue forming a so-called interzone with specific chemical and structural properties.
The combination of different analytical X-ray methods at synchrotrons and in the laboratory en-ables an extensive structural and elemental investigation of such interzones. Within two DFG funded projects, we develop adapted methodologies and investigate micro-chemical changes in interzones which we hypothesize may lead to degradations in the dentine.

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Presenter: MANTOUVALOU, Ioanna (Helmholtz-Zentrum Berlin)

Session Classification: Poster Session 3

Contribution ID: **136** Type: **Poster**

Demonstration of an X-ray Raman Spectroscopy setup to study warm dense carbon at the HED Instrument of European XFEL

Wednesday, November 24, 2021 1:30 PM (1h 40m)

A proof-of-principle study is presented demonstrating X-ray Raman spectroscopy (XRS) from carbon samples at ambient conditions, performed at the High-Energy-Density (HED) instrument of the European X-ray Free Electron Laser.
XRS can provide equivalent information as X-ray absorption spectroscopy (XAS), but overcomes the difficulties in XAS transmission measurements on low-Z materials, that would require, due to their low K-edge energies, the use of soft X-rays and therefore thin targets. XRS, investigating the spectrum of the energy loss of the X-ray photons, can be performed with hard X-rays on bulk targets that are required for shock compression experiments.
The presented setup achieves sufficient spectral resolution and signal strengths to identify the local structure and chemical bonding of diamond and graphite samples. It allows simultaneous implementation of several different diagnostic methods, that are routinely used in warm dense matter experiments, and will enable accurate XRS measurements in upcoming pump-probe experiments with high repetition-rate.

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Session Classi ication: Poster Session 3

Contribution ID: **137** Type: **Poster**

Development of a High-Power Density Neutron Target - Design and first Experimental Tests

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The interest in accelerator-driven neutron sources has increased worldwide, especially with regard to the increasing shutdown of existing fission-based neutron sources.

Within the framework of the Jülich High Brilliance Neutron Source (HBS) project, a compact high-flux accelerator-based neutron source that has the potential to replace current national fission-based neutron sources is developed. One of the key components as well as the main power-limiting factor is the neutron target. Unique requirements specified for the target are given by a 70 MeV pulsed proton beam with a peak current of 100 mA and an average thermal power of 100 kW on a target area of 100 cm^2.

A first tantalum target prototype with an innovative micro channel cooling structure was developed, manufactured and successfully high heat flux tested at 10 MW/m^2. The specifics of the target cooling as well as the results of experimental heat load and erosion tests will be presented.

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Session Classi ication: Poster Session 3

Contribution ID: **138** Type: **Poster**

RAIRS study of low temperature formic acid adsorption on Cu nanoparticles on vicinal (10-14) ZnO

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We studied the low temperature adsorption of formic acid on molecular beam epitaxy grown Cu nanoparticles on stepped, vicinal (10-14) ZnO surfaces by polarized reflection–absorption infrared spectroscopy (RAIRS). Our results clearly show, that the Cu nanoparticles greatly facilitate the deprotonation of formic acid compared to pure ZnO. The dissociated formate species are adsorbed on different facets of the Cu nanoparticles in both mono- and bi-dentate binding geometries. The comparison of p- and s-polarized RAIRS measurements hints towards a binding of the formate species perpendicular to the ZnO steps, which are arranged at an angle of 24.8° to the ZnO(10-14) surface normal.

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Session Classi ication: Poster Session 3

Contribution ID: **139** Type: **Poster**

HILITE - stored ions for non-linear laser-ion experiments

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Free-electron lasers with photon energies in the XUV to X-ray regime open up new possibilities to investigate nonlinear laser-matter interaction. Ionic systems with one active electron are of particular interest.

To investigate such systems, we have built and operated the HILITE (High-Intensity Laser Ion-Trap Experiment) Penning trap. The ions are produced by an EBIT and captured dynamically in the trap centre. We have stored highly charged ions for several minutes and have been able to observe them non-destructively. Last year, we have operated our setup at the FLASH2 laser facility at DESY, with the aim of investigating two-photon ionisation of O⁵⁺ at photon energies of 80 eV and intensities of 10¹⁶W/cm².

We will present the setup and results of this first beamtime. We will also present upgrades of the setup and our planned beamtime at the JETI200 laser in Jena, which will focus on field ionisation of hydrogen-like ions.

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Session Classi ication: Poster Session 3

Contribution ID: **140** Type: **Poster**

Emergent phenomena in topological quantum materials: from single-crystal growth to neutron scattering

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Recent theoretical predictions and experimental realizations of exotic fermions and topologically protected phases in condensed matter have led to tremendous research interests in topological quantum materials, such as magnetic Dirac and Weyl semimetals, and intrinsic magnetic topological insulators etc. In this poster, we will present our recent activities on the single-crystal growth and neutron scattering studies of topological quantum materials, including magnetic Dirac semimetal $EuMnBi_2$ [1] and topological magnon insulators in two-dimensional van der Waals ferromagnets $CrSiTe_3$ and $CrGeTe_3$ [2].

[1] Fengfeng Zhu, *et al.*, Phys. Rev. Research **2**, 043100 (2020).
[2] Fengfeng Zhu, *et al.*, Sci. Adv. **7**, eabi7532 (2021).

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Session Classification: Poster Session 3

Contribution ID: **141** Type: **Poster**

Magnetic properties of nitrogen doped red diamond

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The magnetization of crystalline red diamond bulk samples were investigated in the temperature range between 2 K and 125 K and at applied magnetic field up to ±7 T. The investigated diamond samples are of type Ib with a nitrogen content less than 200 ppm, displaying a yellow color. They were transformed to red color diamonds after irradiation with 10 MeV electrons at T = 900℃, in vacuum, owing to the formation of nitrogen-vacancy centers. Field dependent magnetization, m(H), measurements for temperatures T<10 K show unusual hysteresis loops, which we interpret as consequence of the superposition of coexisting superconducting and paramagnetic regions present in the sample. Temperature dependence of the magnetization, m(T), measured in the zero magnetic field and field-cooled mode shows a paramagnetic behavior accompanied with an irreversibility for T < 13 K, while at higher temperatures a diamagnetic behavior, similar to undoped diamond is observed.

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Session Classification: Poster Session 3

Contribution ID: **142** Type: **Poster**

Reconstructing the plasma temperature by optical probing method in femtosecond laser hydrogen jet interaction and benchmark to the PIC simulation

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Plasma temperature is a critical parameter in warm dense matter and unable to be measured directly. In this study, we apply a well-designed experiment to generate an adiabatic expanded, thermalized hydrogen plasma in few ps by 30fs 1.63e18W/cm2 short pulse laser and 5um diameter solid hydrogen jet interaction. With the optical laser probing method at different wave length, the plasma density in expansion process is recorded with optical shadow image. Then plasma temperature is reconstructed by finding the best fit between experiment and hydro with ray tracing simulations. The electron temperature is determined to be around 300eV through this method and compared to the PIC simulations. The results show that both PIConGPU and PICLS overestimate the electron temperature several factors. This is the first time that we design an experiment and benchmark to the PIC codes. The result would help us improve the existed laser plasma interaction model in PIC.

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Session Classi ication: Poster Session 3

Contribution ID: **145** Type: **Poster**

High-Resolution Microcalorimeter Measurement of X-Ray Transitions in He-like Uranium at CRYRING@ESR

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We present the first application of metallic magnetic calorimeter detectors for high resolution X-ray spectroscopy at the electron cooler of CRYRING@ESR, the low energy storage ring of GSI, Darmstadt. Within the experiment, X-ray radiation emitted as a result of recombination events between the cooler electrons and a stored beam of U^{91+} ions was studied. For this purpose, two maXs detectors were positioned under observation angles of 0 and 180 with respect to the ion beam axis. This report will focus on details of the experimental setup, its performance and its integration into the storage ring environment. This research has been conducted in the framework of the SPARC collaboration, experiment E138 of FAIR Phase-0 supported by GSI.
We acknowledge substantial support by ErUM-FSP APPA (BMBF n 05P19SJFAA).

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Session Classi ication: Poster Session 3

Contribution ID: **146** Type: **Poster**

Incommensurate noncolinear magnetic structures in EuPtAs

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Magnetic systems lacking inversion symmetry and with significant spin-orbit coupling can exhibit the aymmetric Dzyaloshinskii-Moriya (DM) exchange interaction between magnetic moments, in addition to the Heisenberg-type exchange interactions, which can give rise to a number of complex non-collinear magnetic ground states[1], such as helical magnetic structures. We have recently characterized the magnetic properties and phase diagram of EuPtAs, which is isostructural to CeAlGe [7]. Using x-ray resonant magnetic scattering (XRMS) at P09/PETRA III of DESY, we have studied the magnetic structures in different phases. Our results suggest that EuPtAs exhibits incommensurate magnetic structure below TN followed by a lock-in transition at TM. Together with the neutron scattering measurements, our preliminary studies indicate noncolinear magnetic structure in EuPtAs at zero field, while the studies in magnetic fields applied in different directions, especially the search for potential TST, are still underway.

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Session Classification: Poster Session 3

Contribution ID: **147** Type: **Poster**

A pipeline for a three-dimensional X-ray phase contrast Xenopus laevis atlas and its opportunities for research

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The African clawed frog (Xenopus laevis) is an important vertebrate model organism to study development and disease. In 1991 a 2D light microscopy atlas of sectioned opaque embryos of different developmental stages was published. It still serves as the frame for the comparison of morphological data during embryogenesis.
Today using synchrotron X-ray phase-contrast microtomography in combination with a new staining protocol the limitations of light microscopy can be circumvented and 3D high-detail whole embryo tomographic data can be created.
Here we present the full pipeline including sample fixation, data acquisition and optimized post-processing. We show several highlights of the 3D morphology and emphasize the functions of the localization of different cell types and developing organs. This will considerably complement the existing 2D atlas and provide the community with an easily accessible, fully comparable protocol for inter laboratory data and broaden our understanding of gene functions, mutations and environmental factors.

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Session Classification: Poster Session 3

Contribution ID: **148** Type: **Poster**

eCOMO — A new endstation for controlled molecule experiments

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We present details on our newly established transportable endstation eCOMO (Endstation for Controlled Molecules). The apparatus has been designed for use at various photon sources for investigating the molecular dynamics of small molecules in the gas phase [1].

The endstation consists of three main parts: 1) An Even-Lavie-valve-based gas source. 2) An electrostatic deflector for the generation of pure molecular samples [2-3]. 3) A double-sided VMI spectrometer coupled with the time- and position-sensitive Timepix3 detector and the pymepix data acquisition and analysis software [4-5].

The endstation was designed to be highly transportable, with built-in transport wheels, adjustable height, integrated controllers, power supplies as well as water and gas lines for easy beamtime installation.

In collaboration with the Group of Francesca Calgary, within the Center for Molecular Water Science, We found a novel decay with a damped oscillation in ionization dynamics of OCS. The results will be discussed on the poster.

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Session Classi ication: Poster Session 3

Contribution ID: **149** Type: **Poster**

3D X-ray Diffraction Microscopy (3DXRD) Using High Resolution X-ray Nanodiffraction

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The existing technology called 3D X-ray diffraction microscopy (3DXRD) is a well-established technique to map the grain structure of polycrystalline systems. It is based on reconstruction algorithms which trace the positions of multiple Bragg-Peaks as a function of the rotation angle during the rotation of the sample. Due to a given beam size and limits of the reconstruction software only a certain number of grains can be tracked, resulting in a minimum mappable grain size.

The newly implemented experiment uses a nano-focused synchrotron beam (e.g. Nanofocus Endstation of P03, PETRA III at DESY) to examine very fine-grained systems. The small beam size allows detecting grains below the size limit of standard 3DXRD.

First reconstructions of the most recent experiment as well as the experimental setup, which was developed to ensure a stable and precise rotation, will be presented. The results include an outlook of future strain analyses.

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Session Classification: Poster Session 3

Contribution ID: **150** Type: **Poster**

Polarization transfer in hard x-ray Rayleigh scattering for non-zero azimuthal scattering angles

Wednesday, November 24, 2021 1:30 PM (1h 40m)

For photon energies up to the MeV range, Rayleigh scattering is the dominant contribution to elastic scattering of x-rays on atoms. This 2nd order QED process of a photon being scattered on a bound electron exhibits a high degree of sensitivity to the polarization characteristics of the incoming photons. Measurements precisely determining the polarization of the incident and the outgoing photon are therefore suitable for the most stringent tests of the underlying theory.
We performed an experiment at the synchrotron facility PETRA III of DESY, Hamburg, scattering highly linearly polarized x-rays with a photon energy of 175 keV on a gold foil. Using a prototype 2D-sensitive silicon strip detector developed within the SPARC collaboration as Compton polarimeter, we analyzed the polarization characteristics of the scattered beam both within and out of the polarization plane of the incident photon beam. We will present experimental details and first results of this beamtime.

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Session Classification: Poster Session 3

Contribution ID: **151** Type: **Poster**

Phase Changes in Dynamically Compressed Water

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Extreme conditions are ubiquitous in nature. Of interest, are the planetary interiors of the icy giants, Uranus, and Neptune. Which are understood to contain mixtures of water, ammonia, and hydrocarbons ices. High pressure ice above ~1500K and 50 GPa is predicted to undergo a superionic transition. These superionic phases are a possible source of the complex magnetic fields of both Uranus and Neptune.
Experiments carried out at the LCLS XFEL, used reverberating shocks to compress liquid water to states in the superionic region of the ice phase diagram. The identified phases include previously identified ices, with misfits in the highest-pressure data suggesting the presence of a new phase. Ongoing work aims to determine these structures of ice under superionic P-T conditions and with comparison with simulation, understand the magnetic field behaviour of icy giant type planets.

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Session Classification: Poster Session 3

Contribution ID: **152** Type: **Poster**

Complex quantum dots in III-As nanowires

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Single quantum dots embedded in the core of freestanding semiconductor nanowires grown directly on Si offer a novel and promising scheme for the realization of on-demand sources of single photons or entangled photon pairs in quantum technology systems. The primary challenge in using the nanowire growth medium lies in reducing the compositional grading effect of the axial barrier's constituent materials.
Here, we have investigated the Ga-catalyzed vapor-liquid-solid growth mechanism and optical properties of axial GaAs quantum dots confined between two Al(x)Ga(1-x)As/Al(y)Ga(1-y)As short-period superlattices inside GaAs/In(x)Al(1-x)As and GaAs/Al(x)Ga(1-x)As core/shell nanowires. By increasing the interfacial abruptness between the axial barrier and quantum dot, its relevance was highlighted by significant improvements in the quantum dot emission linewidth. Using tensile strain, the tuneabilty of the quantum dot emission energy was clearly demonstrated across a wide range of wavelengths by employing lattice mismatched InxAl1-xAs shells as radial barriers, showing the potential for telecom band access.

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Session Classi ication: Poster Session 3

Contribution ID: **153** Type: **Poster**

Multilayer Laue lenses for hard X-Rays

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Multilayer Laue lenses (MLL) are volume diffractive optics that are highly efficient at focusing light in the hard X-ray regime. The design, multilayer deposition, lens fabrication, and characterization of MLLs will be presented. We recently built up a new lab facility to characterize the wavefront aberrations of MLLs, using a wavefront sensing methodology we developed called speckle tracking ptychography. These capabilities accelerated our MLLs development and led to better understanding of the origin of the errors as well as enabled us to implement corrections into the fabrication process. Some of the lenses were also measured at the PETRA III synchrotron so we could make a comparison with the results obtained with our laboratory source. The progress in MLL development is remarkable. Recent improvements led to 2D focusing to a spot below 5 nm at 17.5 keV.

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Presenter: DRESSELHAUS, Jan Lukas

Session Classification: Poster Session 3

Contribution ID: **154** Type: **Poster**

Scanning Compton X-ray microscopy

Wednesday, November 24, 2021 1:30 PM (1h 40m)

High-resolution imaging of biological materials is limited by the dose, and hence the exposure, that such materials can tolerate before the structure under investigation is damaged. Higher resolution obviously requires a higher exposure but the exposure needed to record an image at a given signal to noise ratio depends on the contrast mechanism that is exploited. We recently proposed the method of scanning Compton X-ray microscopy at a photon energy of 60 keV as a means to achieve the lowest dose per resolution for biological objects.

Scanning Compton microscopy is made possible with the development of multilayer Laue lenses to produce a focal spot through which the object is scanned. We find that such optics have a diffraction efficiency approaching 90% at 60 keV. We present images of a number of biological samples we collected at the P07 beamline at PETRA III. No samples showed any traces of radiation damage.

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Presenters: IVANOV, Nikolay (DESY); LI, Tang (Centre for Ultrafast Imaging, Hamburg University)

Session Classification: Poster Session 3

Contribution ID: **156** Type: **Poster**

Multimodal spectroscopy with upgraded TRIXS end-station at FLASH

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We report on the capabilities of an upgraded time-resolved resonant inelastic X-ray scattering (TRIXS) end-station at the PG1 monochromator beamline of the free-electron laser FLASH. The new chamber is compatible with the existing TRIXS spectrometer , for the RIXS measurement in the range of 35-200 eV. The setup is equipped with the necessary diagnostics to establish a temporal overlap between an optical laser (at 1030 nm fundamental + harmonics) and the FEL with sub-picosecond resolution. The presence of variety of detection scheme and sample manipulation possibilities will allow us to perform time-resolved soft X-ray absorption (XAS) and soft X-ray reflectivity (SXR) on solid samples once the goals of FLASH2020+ project are achieved. Thus, the upgradation of this chamber with cryostat combined, opens up new possibilities to explore dynamics of phase transitions and novel functionalities of different heterostructures, superlattices or multilayered, correlated electron systems with the help of multi-modal techniques.

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Presenter: SINHA, Mangalika (DESY)

Session Classification: Poster Session 3

Contribution ID: **158** Type: **Poster**

Soft X-ray microscopy to characterise plasma surface modification

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We present the results of an x-ray ptychography experiment at the FLASH2 facility to systematically characterise the morphology of cold-plasma treated polymers. Polymers are often used in industry because of their bulk properties, such as strength and good resistance to chemicals. Due to low surface energy, their surface properties need modification. Plasma surface modification has been widely applied on polymers with success in past decades. Morphological characterisation of surface modification is central to interpreting the influence of plasma treatment on polymers. We address this need with soft x-ray ptychography at free-electron lasers (FELs). X-ray ptychography is a scanning microscopy technique for studying the structure of large-extent samples. A high degree of transverse coherence and unprecedented photon flux make FELs ideal facilities for ptychography.

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Session Classification: Poster Session 3

Contribution ID: **159** Type: **Poster**

Measurement of Spin Dynamics in a Layered Nickelate Using X-Ray Photon Correlation Spectroscopy: Evidence for Intrinsic Destabilization of Incommensurate Stripes at Low Temperatures

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We study the temporal stability of stripe-type spin order in a layered nickelate with x-ray photon correlation spectroscopy and observe fluctuations on timescales of tens of minutes over a wide temperature range. These fluctuations show an anomalous temperature dependence: they slow down at intermediate temperatures and speed up on both heating and cooling. This behavior appears to be directly connected with spatial correlations: stripes fluctuate slowly when stripe correlation lengths are large and become faster when spatial correlations decrease. A low-temperature decay of nickelate stripe correlations, reminiscent of what occurs in cuprates as a result of a competition between stripes and superconductivity, hence occurs via loss of both spatial and temporal correlations

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Session Classi ication: Poster Session 3

Contribution ID: **160** Type: **Poster**

Creation and analysis of artificial radiography images for experiments to investigate the radiation transport in the interior of red dwarfs

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Red dwarfs (M-class stars) are the most abundant and oldest stars in our solar neighborhood. While convection is believed to be the predominant energy transport mechanism within those objects, the opacity - mainly caused by free-free transitions - determines the efficiency of radiation transfer and is therefore a crucial parameter for modelling red dwarfs. In an experiment within the Discovery Science Program of the National Ignition Facility, we intend to compress hydrogen to ≈ 800 times solid density at temperatures around 200 eV. These conditions are directly relevant to the interiors of small stars. We will conduct an opacity measurement using x-ray radiography. In this poster we present simulated detector images, generated to estimate the planned experiment's resolution, to tune parameters and to provide impulses for the analysis of the data that will be acquired in the spring of next year.

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Session Classi ication: Poster Session 3

Contribution ID: **161** Type: **Poster**

Precision References for the Interpretation of Astronomoical X-Ray Spectra

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The next generation of x-ray satellites will be equipped with state-of-the-art spectroscopic instrumentation. However, the accuray of plasma parameters that can be extracted from high-resolution spectra will be limited by the uncertainties and availability of atomic data, especially for highly charged ions. We pursue two complementary approaches to laboratory x-ray spectroscopy, to provide transition energies, rates, and branching ratios for astrophysical applications. On one side, we employ microcalorimeter x-ray detectors, recording x-ray fluorescence spectra with resolving powers similar to satellite instruments. We present an upcoming experiment at the CRYRING storage ring, in which we will study x-ray fluorescence cascades during the relaxation of ions with inner-shell vacancies. On the other side, we use an EBIT to provide targets of highly charged ions for ultrabrilliant x-ray photon beams from synchrotrons and FEL light sources. We present results of resonant-photoexcitation experiments conducted at synchrotron facilities, as well as planned future measurements.

Primary author: BERNITT, Sonja (HI Jena)

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Presenter: BERNITT, Sonja (HI Jena)

Session Classification: Poster Session 3

Contribution ID: **162** Type: **Poster**

The IMAGE beamline at the KIT synchrotron light source

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The work introduces the status and the perspectives of the KIT IMAGE beamline, devoted to full-field hard X-ray imaging applications in Materials and Life Sciences. IMAGE aims at performing systematic in situ and operando studies as well as high throughput investigations based on radiography, tomography, and laminography.
The beamline can provide both white and monochromatised (DMM, DCM) X-ray beams. The white beam allows investigating processes, which require high speed data acquisition, e.g. in situ 4D imaging (Laminography and Tomography), high throughput imaging. The pink beam delivered from the DMM (energy bandwidth ~2%) is suited for phase contrast imaging with spatial resolution up to 1 m. Finally, the monochromatic mode is based on X-ray photons delivered from a Si111 DCM.
In this work the layout of the beamline optics and diagnostics is described. Further, example of applications are shown including monochromatic Bragg magnifier tests in microscopy and conditioning modes experiments.

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Presenter: CECILIA, Angelica (KIT/IPS)

Session Classification: Poster Session 3

Contribution ID: **163** Type: **Poster**

Novel Opportunities to study Dynamics @High Current Accelerator driven Neutron Sources

Wednesday, November 24, 2021 1:30 PM (1h 40m)

At present strong research activities address the development of accelerator driven neutron sources that employ low energy nuclear reactions. Despite the lower neutron yield of the reaction compared to spallation or nuclear fission, the reduced requirements on the accelerator design provide an increased flexibility in terms of source frequency and pulse length. The softer primary neutron spectrum as compared to spallation allows an excellent coupling of primary neutrons into thermal and cryogenic moderators by matching the moderation and storage time constants to the proton pulse length.
For the spectrometer design these features provide an additional degree of freedom. Some concepts that profit particularly will be discussed. I consider in particular instruments that require a limited primary bandwidth, which can be offered efficiently by a high frequency pulsed neutron source.

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Presenter: VOIGT, Jörg (Forschungszentrum Jülich)

Session Classification: Poster Session 3

Contribution ID: **164** Type: **Poster**

Modeling of magnetization decrease in cobalt under soft X-ray radiation

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We report on preliminary results obtained with the modeling tool XSPIN constructed to describe ultrafast demagnetization induced by X-ray free-electron laser radiation in ferromagnetic materials. It combines the ab initio description of the material (electronic structure), and Monte Carlo approach to X-ray/XUV-induced collisional processes in the material (photoionization from core and valence levels, Auger decay and fluorescence; electron scattering, including impact ionization and intraband (elastic) scattering) adopted from XTANT code [Medv13,Medv18a,Medv18b]. We analyzed the experimentally investigated evolution of magnetic systems irradiated with X-rays of different wavelengths. These are the recent mSAXS data from magnetic multilayer systems recorded at M-edge of Co (photon energy~60eV)[Kobs20], and at L-edge of Co (photon energy~778eV)[Wu16]. Our results show that the magnetic scattering signal decreases with the increasing fluence of the incoming radiation, following the trends observed in the experiments.

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[Wu16]B.Wu,et.al., Phys.Rev.Lett. 117,027401(2016).

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Session Classification: Poster Session 3

Contribution ID: **166** Type: **Poster**

Using Alphafold2 and MHz SFX to solve the structures of bacterial insecticides.

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Bacterial insecticides from Bacillus thuringiensis can specifically target e.g. agricultural pests, but do not harm other insects and are safe for higher organisms. Using such insecticides for agricultural purposes instead of chemical agents will help to stop the decline in insect populations across the globe. Insecticides that target mosquito larvae can be used to fight the spread of e.g. Zika and Dengue virus and other pathogens for which mosquitoes act as vectors. These proteins natively form in vivo grown nanocrystals that are ideal candidates for SFX at XFELs. For many of these proteins no structural homologues exist in the protein data base, rendering phasing with molecular replacement impossible. We used an installation of Alphafold2 at DESY and the Maxwell cluster to predict models and the data from MHz SFX at EuXFEL to elucidate the structures of nanocrystalline insecticides.

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Presenter: OBERTHÜR, Dominik (DESY)

Session Classification: Poster Session 3

Contribution ID: **168** Type: **Poster**

Cold moderator developments for the prototype of the High Brilliance Neutron Source

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Currently, two different cold neutron moderator systems for the planned prototype of a Target-Moderator-Reflector (TMR) unit of the HBS are being manufactured at Forschungszentrum Jülich: one for liquid para-hydrogen (l-pH2) and the other for solid methane (s-CH4). While the l-pH2 system allows a continuous closed-cycle operation with the l-pH2 acting both as neutron moderator and coolant, the s-CH4 system is operated in a discontinuous batch-style with periodic filling/emptying of the moderator vessel, using a separate flow of liquid helium as coolant.
Positioning inside the TMR unit is realized by using a so-called "moderator plug", including a cryostat that allows the exchange and testing of different moderator vessels. Additionally, the s-CH4 system consists of a gas-management-panel, whereas the p-H2 moderator will comprise a main cryostat that is connected to the moderator plug via a vacuum-insulated, adjustable connector. Commissioning and extensive testing of these systems is planned for summer of 2022.

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Presenter: SCHWAB, Alexander

Session Classification: Poster Session 3

Contribution ID: **169** Type: **Poster**

Target / Moderator / reflector concepts for a compact accelerator-based neutron source

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Compact high-current accelerator-based neutron sources provide a competitive and cost-efficient option for the neutron production alternative to spallation or fission. Such sources are scalable and allow the operation of multiple target / moderator / reflector assemblies (TMR) simultaneously providing neutron beams with a specific energy spectrum and pulse structure. This flexibility in operation parameters allows optimizing the TMR unit regarding its material and geometry to a specific set of neutron scattering instruments maximizing the usable brilliance and therefore the flux at the sample position.

We will present different concepts of a TMR unit planed for the High-Brilliance neutron Source (HBS) project operated at pulse frequencies of 24 Hz and 96 Hz.

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Presenter: ZAKALEK, Paul (JCNS-HBS, Forschungszentrum Jülich GmbH)

Session Classification: Poster Session 3

Contribution ID: **170** Type: **Poster**

Measurement of Magnetic Moments in Heavy, Highly Charged Ions Using Laser-Microwave Double-Resonance Spectroscopy in ARTEMIS at HITRAP

Wednesday, November 24, 2021 1:30 PM (1h 40m)

In ARTEMIS (AsymmetRic Trap for measurement of Electron Magnetic moment in IonS), at HITRAP, we aim to perform the g-factor measurements of medium to heavy highly charged ions, such as 209Bi82+. It serves as a test of QED in strong fields and we do this using laser-microwave double-resonance spectroscopy. The setup includes a Creation Trap which i) acts as a mini-EBIT for the in-situ production of ions and also ii) allows for inflight capture of ions. We store ions for a few weeks (currently-argon) and cool them resistively. This uses the interaction of the induced current from the ions with the effective resistance offered by the RLC detection system made of copper/NbTi resonators to non-destructively detect the ions. We have received ions in the final Faraday cup of the vertical beamline and the remaining construction to connect ARTEMIS with HITRAP is in sync with the proposed beamtime of May 2022.

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Session Classification: Poster Session 3

Contribution ID: **171** Type: **Poster**

Characteristics of the Jülich High Brilliance Neutron Source (HBS) in instrument simulation software

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Based on MCNP simulations of a simplified target-moderator-reflector (TMR) system, the source characteristics of the Jülich High Brilliance Neutron Source (HBS) [1] have been modeled to be used in the instrument simulation packages VITESS [2] and McStas [3]. According to the variable neutron source, the simulation code contains several variable parameters: source frequency, proton pulse length, time constants of the pulse shape, moderator geometry and temperature dependence of the flux. This also enables adaptions to updates of the source characteristics due to improved simulations ot the TMR system. This code will be used to simulate all instruments that will be suggested in the Technical Design Report of the HBS. It is released in McStas 2.7.1 and will be released with the upcoming version VITESS 3.5, but is already available from the developer team.

[1] T. Gutberlet et al., Phys B Condens Matter 570 (2019) 345–348.
[2] https://www.helmholtz-berlin.de/vitess
[3] www.mcstas.org

Primary authors: LIEUTENANT, Klaus (Forschungszentrum Jülich); Mrs BÖHM, Sarah (RWTH Aachen); LI, Jingjing (Forschungszentrum Jülich GmbH); ZAKALEK, Paul (Fosrchungszentrum Jülich GmbH); Dr VOIGT, Jörg (Jülich Centre for Neutron Science and Peter Grünberg Institute, JARA-FIT, Forschungszentrum Jülich GmbH)

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Session Classification: Poster Session 3

Contribution ID: **172** Type: **Poster**

Optimized thermal moderators for HBS-type neutron sources

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The thermal moderators of a low-energy accelerator driven neutron source, as e.g. HBS, are needed to moderate the primary neutrons emitted from the target, typically with MeV energies, down to meV energies where they are useful for the investigation of solid matter. The target typically has a volume well below 1 dm^3, and a suitable moderator (and reflector) design must keep the neutron cloud inside a volume of comparable size to allow the extraction of high-brilliance thermal neutron beams.
On this poster, we will present which influence the choice of geometry and materials has on the spatial distribution of thermal neutrons and on the time structure of the neutron pulse. Different assemblies will be proposed suitable for long-pulse and for intermediate-pulse instruments. The problems to supply intense, but sufficiently short neutron pulses for instruments with a high repetition rate will be discussed.

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Session Classification: Poster Session 3

Contribution ID: **174** Type: **Poster**

Deep Learning for X-ray Imaging applications at KARA synchrotron

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Deep learning(DL) is emerging as the leading machine learning tool in imaging and computervision. Recent results indicate that the generic descriptors extracted fromdeep convolutional neural networks (CNN) are extremely effective in object andpatterns recognition. Here we present a number of applications for X-ray Imaging problems: 1) laminographic artifacts reduction (due to the incomplete sampling of the Fourier space); 2) ring artifacts removal from tomographic images (due to the imperfections in optical elements and beam fluctuations) 3) automated segmentation of morphological structures in tomographic images of model organisms and 4) self-supervised learning techniques for automated object localization and cropping (data reduction). We also outline a number of promising techniques which are currently in development at the Imaging group of the KARA synchrotron.

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Presenter: ERSHOV, Aleksei (Karlsruhe Institute of Technology (KIT))

Session Classification: Poster Session 3

Contribution ID: **175** Type: **Poster**

Convergent beam X-ray crystallography and 3-D diffraction microscopy

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Highly-converging X-ray beams created by multilayer Laue lenses(MLLs) bring new opportunities for crystallography and 3D diffraction microscopy. Our recent MLLs achieve a numerical aperture of 0.03 at a photon energy of 17 keV, with an angular range of 60 mrad(3.4°). This angle is considerably greater than the spacing of Bragg peaks in most protein crystals. When a crystal is placed near the focus, Bragg peaks overlap and interfere to provide phase information. However, when the crystal is placed far from focus, there is a correlation between position in the beam and the X-ray incidence angle. In this configuration, the diffraction data provides a mix of crystallography and (tomographic) microscopy.We are interested in developing convergent-beam-diffraction as a way to obtain fully-integrated Bragg reflections in single exposures and to obtain structure factors of high accuracy by accounting for spatial variations in crystals, such as their shape, strain, or defect structure.

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Presenter: LI, Chufeng (DESY CFEL)

Session Classification: Poster Session 3

Contribution ID: **177** Type: **Poster**

High-power and High-energy cryogenic lasers

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We present our efforts in high-power and high-energy cryogenic laser development to address the need for sub-joule to joule laser pulses at a high repetition rate to laser applications in laser-driven electron acceleration, laser diagnostics, and THz acceleration. The demonstrated Yb: YLF and Yb: YAG lasers provide hundreds of millijoule to joule output energies at cryogenic temperatures (78K). Specifically, prototypes of those laser systems with output parameters of 1 joule at 500Hz and 100 mJ at 1kHz are shown. We discuss further possibilities to increase the output parameters as well as IR laser (2 um) implementations.

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Presenter: PERGAMENT, Mikhail (Deutsches Elektronen Synchrotron (DESY))

Session Classification: Poster Session 3

Contribution ID: **178** Type: **Poster**

Ultrafast melting of Warm Dense Cu studied by x-ray spectroscopy

Wednesday, November 24, 2021 1:30 PM (1h 40m)

We present a study of ultra fast heating of Warm Dense Cu diagnosed by means of x-ray absorption spectroscopy carried at the Draco laser facility at HZDR. A thin Cu foil is directly heated to few eV temperature by an ultra-short laser pulse (40 fs, 1 J) and probed variable delay later (between 0.2 and 20 ps) by a laser-driven betatron radiation. This betatron radiation, created by a laser wakefield accelerator, is an unique x-ray source with its ultra short duration and broadband spectrum. The shift and broadening of the K edge is showing the evolution of the electron temperature, while the decay and transformation of the EXAFS oscillatory peaks (Extended X-ray Absorption Fine Structure) is showing the decay of the crystallite structure. The data are evaluated by using analytical models and numerical DFT-MD simulations. Both diagnostics together demonstrate the complex nature of ultra-fast melting processes and creation of WDM.

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Presenter: ŠMÍD, Michal (HZDR)

Session Classification: Poster Session 3

Contribution ID: **180** Type: **Poster**

Terahertz-Based Electron Acceleration for AXSIS

Wednesday, November 24, 2021 1:30 PM (1h 40m)

AXSIS is a concept for a compact attosecond X-ray source to probe biological molecular processes on the fastest timescales. AXSIS employs a novel approach to electron acceleration and manipulation based on laser-generated terahertz radiation whose short wavelengths and pulse durations enable construction of millimeter-scale structures with extreme fields. By sending the THz-accelerated electrons into a laser-powered optical undulator, few-keV X-rays can be generated with expected pulse durations below 1 femtosecond and intrinsic synchronization to the laser system. A dedicated facility has been constructed and proof-of-principle experiments have demonstrated the viability of the terahertz approach. Construction of the first AXSIS prototype is currently under way and expected to be complete within the next year. In parallel, application of the THz-enhanced electron sources to the measurement of atomic-scale dynamics using ultrafast electron diffraction has also been successfully demonstrated. The combined laser, electron and X-ray resources will make AXSIS a unique facility.

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Presenter: MATLIS, Nicholas (DESY (Deutches Elektronen Synchrotron))

Session Classification: Poster Session 3

Contribution ID: **181** Type: **Poster**

Simulation of laser-driven multi-cycle terahertz generation in nonlinear crystals

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Employing high-field pulses of multi-cycle terahertz (MC-THz) radiation for linear electron acceleration promises miniaturization of accelerators opening up new realms of applications of electron sources. Pulses with energy of 20-40 mJ are needed for effective THz acceleration.
We explore different ways to overcome the Manley-Rowe limit for THz generation with nonlinear down-conversion of infrared (IR) laser radiation by cascading in periodically poled nonlinear materials. Due to limitations by laser induced damage, conversion efficiencies beyond several percent from IR to THz are required.
Numerical simulations of the nonlinear cascading process including pump depletion and relevant nonlinear effects are conducted to optimize MC-THz generation with IR pulse trains. Internal conversion efficiencies of about 2.5 % are predicted under assumption of realistic conditions. Further concepts of THz generation like recycling the cascaded IR output and modulation of a strong laser line with either a THz seed or a cascaded IR field are investigated.

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Presenter: RENTSCHLER, Christian (DESY)

Session Classification: Poster Session 3

Contribution ID: **182** Type: **Poster**

Small compound crystal screening with SARS-CoV-2 methyltransferases

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Non-structural protein 10 (nsp10), nsp14, and nsp16 are part of the RNA synthesis complex which is crucial for viral replication in SARS-CoV-2. It has been shown that inactivation of these proteins interferes severely with viral replication, making them promising drug targets against COVID-19. As only limited information on ligands binding to nsp10-nsp16 is available, we focus on testing small compound libraries (< 200 compounds) via X-ray crystallography that where soaked into protein crystals and have a high chance to contain potential binders. To this point, we obtained data sets of the nsp10-16 complex interacting with derivatives of the native methyltransferase substrate with the nsp16 active sites. Promising compounds will be further tested in binding and activity assays. In parallel, nsp14 will be screened in the same way since the enzymatic activity is similar to nsp16. Our results may contain binders that can serve as novel drugs against COVID-19.

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Presenters: KREMLING, Viviane (DESY, FS-CFEL-1); SPRENGER, Janina (DESY, FS-CFEL-1)

Session Classification: Poster Session 3

Contribution ID: **183** Type: **Poster**

Compact Photogun Transversely Pumped by Twin Single-Cycle Terahertz Pulses

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Novel accelerator concepts such as all-optical terahertz (THz) based compact accelerators promise to enable new science due to unique features such as reduced timing-jitter and improved space charge broadening of the generated electron bunches. However, multi-keV electron photo-guns based on short single-cycle THz pulses for acceleration have not been demonstrated experimentally so far. Here, we present a modular THz-driven electron gun with both tunable interaction length and output orifice allowing optimization of the sub-mm interaction volume. First extraction of multi-keV electrons is demonstrated and the parameter space as well as resulting performance of the THz-driven gun by varying the timing of the two single cycle THz pulses and the UV photo-excitation pulse are explored. Such compact gun prototypes are not only promising as injectors for compact THz-based LINACs but also as source for ultrafast electron diffraction experiments.

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Session Classification: Poster Session 3

Contribution ID: **184** Type: **Poster**

Observing the Oxidation of Platinum under operando Electrochemical Conditions

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Platinum electrocatalyst degradation forms a large barrier for the wide-spread application of electrolysers and fuel cells, which are crucial for a sustainable energy society. Oxidative processes play a major role in this degradation. Therefore, a detailed understanding of the catalyst surface structure under oxidative conditions is required to design more stable catalysts. High-Energy Surface X-Ray Diffraction (HE-SXRD) experiments under static, oxygen-free conditions have provided a detailed description of the initial oxidation of Pt model electrodes.
To improve the understanding of the Pt surface oxidation under operando conditions, we have developed a Rotating Disk Electrode (RDE) setup that enables HE-SXRD experiments while maintaining well-defined diffusion conditions and high catalytic reaction rates (current densities). With this setup we followed the oxidation of Pt(111) and Pt(100) model electrodes, from the Place-Exchange surface oxidation occurring around 1.1V until the formation of a (bulk) disordered oxide at potentials relevant for the oxygen evolution reaction.

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Presenter: JACOBSE, Leon (DESY)

Session Classification: Poster Session 3

Contribution ID: **185** Type: **Poster**

Magnetic doping at the nanoscale: exchange interaction vs Jellium shells

Wednesday, November 24, 2021 1:30 PM (1h 40m)

The interaction of localized spins with free electrons remains an interesting and relevant topic due to not only its fundamental nature but also its implications for quantum technologies such as spintronics. With the aim of studying this interaction with atomic-level control of the size of the free electron gas, we investigated the electronic structure and magnetic properties of free, cobalt-doped, size-selected silver clusters. Using a combination of x-ray magnetic circular dichroism spectroscopy, Stern-Gerlach deflection experiments, density functional theory modeling, and charge-transfer multiplet simulations, we were able to follow how the magnetic impurity reacts as the number of free host-electrons increases one by one.

Primary author: ZAMUDIO-BAYER, Vicente

Presenter: ZAMUDIO-BAYER, Vicente

Session Classification: Poster Session 3

Contribution ID: **187** Type: **Poster**

Baking and Boosting - positrons for high-performance Nb cavities

Wednesday, November 24, 2021 1:30 PM (1h 40m)

In recent years, superconducting radio-frequency cavities have been investigated in their potential as qubits, showing a significantly longer decoherence time compared to other realizations.
Originally, SRF cavities are the workhorse of modern particle accelerators and ongoing R&D tries to increase the accelerating field and reduce the surface resistance to improve the energy reach and duty cycle of accelerators. For both applications, the underlying mechanisms of observed losses have not been well understood.
A recently reported anneal of SRF niobium cavities in a comparable low temperature range reduces the residual surface resistance to unprecedented values and leads to extraordinary performances of the cavities. Dynamic in-situ positron annihilation lifetime spectroscopy showed for the first time that this effect is linked to an important reorganization of the niobium oxide and near-surface vacancy-hydrogen complexes and that this reorganization can explain the observed improved performance in both applications.

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Session Classification: Poster Session 3

Contribution ID: **188** Type: **Poster**

Voltage-driven motion of oxygen and nitrogen ions: role of defects in magneto-ionics

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Nowadays magnetoelectronic devices are still controlled by electric currents, a scheme which suffers from energy losses due to heat dissipation. Employing electrical fields as a substitution of currents can strongly reduce ohmic losses and is expected to be crucial for energy-efficient applications. Here, a voltage-induced ionic motion (magneto-ionics) is proposed to control the magnetic properties. In traditional magneto-ionic systems oxygen or lithium are exploited as transport ions and, only recently, nitrogen. We will demonstrate magneto-ionic effects in single-layer iron and cobalt nitride films. Their microstructural and magnetic properties are evaluated and compared with previously studied oxides using positron annihilation spectroscopy and magnetometry techniques. The electrolyte-gated ionic migration enables switching between paramagnetic and ferromagnetic states. The role of vacancies and their agglomerations at grain boundaries are emphasized as diffusion channels, which allow for a fast migration and large incorporation of the ionic species.

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Session Classi ication: Poster Session 3

Contribution ID: **196** Type: **Poster**

Studying the Chemical and Electronic Structure of Perovskite Solar Cells using Electron and Soft X-Ray Spectroscopy

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Perovskite-based solar cells have attracted enormous interests due the simple processing and high power conversion efficiency. However, low stability under ambient conditions and lead as a main component are detrimental for commercialization. To improve their stability and help in the development of lead-free perovskites, an in-depth knowledge of the chemical and electronic structure of the perovskite thin-films stacks is crucial. In particular, surfaces and interfaces play an important role, which can be studied by surface-sensitive electron spectroscopies (PES) and bulk-sensitive soft x-ray spectroscopies, i.e., x-ray absorption spectroscopy, (XAS), x-ray emission spectroscopy (XES), and resonant inelastic soft x-ray scattering (RIXS).
In this contribution, we use a combination these techniques and give depth-varied insights into the chemical and electronic structure of perovskite precursors *and* stability improving surface treatments.

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Session Classification: Poster Session 3

Contribution ID: **197** Type: **Poster**

Static Density Response of the Warm Dense Electron Gas beyond Linear Response Theory: Excitation of Harmonics.

Wednesday, November 24, 2021 1:30 PM (1h 40m)

Experimental setups as well as theoretical modeling of Warm Dense Matter (WDM) heavily rely on linear response theory. However, Dornheim et. al. [Phys. Rev. Lett.125, 085001 (2020)] showed that assuming the linear regime is not always justified for WDM. We use the ab initio Path-Integral Monte-Carlo (PIMC) technique to obtain exact results for the harmonically perturbed homogeneous electron gas. A thorough analysis for different perturbation amplitudes is carried out. The corresponding density response reveals resonances at higher harmonics of the chosen perturbation frequency. Furthermore, the induced density response as a function of the perturbation strength unveils that the dominant term beyond linear response is the second harmonic. We show that the nonlinear density response is highly sensitive to exchange–correlation effects, rendering it a potentially valuable new diagnostic tool. The results signify the importance of response contributions beyond the linear regime to accurately model WDM.

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Session Classification: Poster Session 3

Contribution ID: **198** Type: **Poster**

X-SPEC: A 70 eV to 15 keV undulator beamline for x-ray and electron spectroscopies

Wednesday, November 24, 2021 1:30 PM (1h 40m)

X-ray and electron spectroscopies are powerful techniques for material characterization, both in fundamental studies as well as for applied systems. In particular, x-ray emission spectroscopy (XES), resonant inelastic x-ray scattering (RIXS), and hard x-ray photoelectron spectroscopy (HAXPES) have seen a significant recent development and create a unique method combination.
X-SPEC is a spectroscopy beamline optimized for these techniques, which has been built, commissioned and is now operated at the KIT (Karlsruhe Institute of Technology) light source. X-SPEC is a high-flux spectroscopy beamline for electron and x-ray spectroscopy, featuring a wide photon energy range. Using a combination of soft and hard x-ray undulator sources and optics, X-SPEC can cover an energy range from 70 eV up to 15 keV at high flux. The beamline offers both UHV as well as in situ and operando conditions. Design considerations, resulting beamline layout, beamline performance, and some first scientific results will be presented.

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Session Classification: Poster Session 3

Contribution ID: **5** Type: **Invited Talk**

Investigations on the kinetics of the liquid-liquid phase separation of myelin basic protein: Combining neutron scattering with imaging techniques

Wednesday, November 24, 2021 3:10 PM (20 minutes)

The myelin basic protein (MBP) is a key player when it comes to the formation of tight membrane wrapping around vertebrate's nerve cells. In physiological conditions, MBP is acting as a glue that stacks multiple myelin layers to build up an insulating sheath which covers axons. To accomplish this task, MBP undergoes a so-called Liquid-Liquid Phase Separation (LLPS) - a property which has recently attracted wide attention in the biological and biophysical community.
Although the importance of its phase-separating ability is already known, the kinetics of MBP's LLPS are not well studied yet. Hence, we focus on investigations that follow the formation of liquid-like MBP droplets which can be observed when suitable conditions are applied. To examine both the nucleation and the growth of those µm-sized condensates, we combine conventional imaging techniques and (neutron) scattering experiments: Confocal / Transmission microscopy, Dynamic light scattering, and (Time resolved) SANS.

Primary author: WESTARP, Igor (JCNS-1)

Presenter: WESTARP, Igor (JCNS-1)

Session Classification: Session I

Contribution ID: **155** Type: **Invited Talk**

High-Throughput Morphological 3D Imaging

Wednesday, November 24, 2021 3:30 PM (20 minutes)

Tomography of fossil, fixed and even living specimens contributes to our understanding of extinct and recent species with high relevance for biomedical research field like evolutionary biology, developmental biology, ecology, functional morphology and medicine. Vertebrate model organisms provide indispensable paradigms to study multigenic contributions to development and disease. And, with their high biodiversity, arthropods such as insects fulfill key functions in our ecosystems. All cases share the need for high-throughput 3D imaging of a huge number of individuals to facilitate systematic quantitative analyses of body, organs, tissues, and cells and their correlation with molecular, genetic, environmental and other information.
We established a broad research network for fast and high-throughput X-ray imaging of small animals and developed dedicated software and instrumentation. The talk will highlight recent methodological developments and scientific results.

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Presenter: VAN DE KAMP, Thomas (Karlsruhe Institute of Technology (KIT))

Session Classification: Session I

Contribution ID: **63** Type: **Invited Talk**

Structural microbiology at the crossroads of bacterial signaling and RNA degradation

Wednesday, November 24, 2021 3:50 PM (20 minutes)

Biofilm formation - the switch from a free-swimming to a sessile, social lifestyle - is a prevalent adaptation mechanism in bacterial physiology. The process enables bacteria to colonize surfaces and provides protection against environmental insult. The commitment to biofilm formation relies on the bacterial second messenger c-di-GMP, enzymes for its synthesis and degradation, and receptors that translate second-messenger levels into physiological responses. Notably, the clearance of c-di-GMP, and in particular its linear di-GMP intermediate, intersects with the general RNA degradation pathway, suggesting a specific cellular function of the enzymes that process the smallest RNA breakdown products. Here, I will present our current understanding of the molecular principles acting at the intersection of c-di-GMP signaling and RNA metabolism. Mechanistic insight may allow us to manipulate bacterial cell adhesion and fitness as strategies against biofilm-dwelling pathogens.

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Session Classification: Session I

Contribution ID: **83** Type: **Invited Talk**

Exploitation of carbon-ion radiotherapy in combination with immunotherapy to tackle metastatic cancer disease – pre-clinical research activities at GSI

Wednesday, November 24, 2021 4:10 PM (20 minutes)

Immunotherapy is a new, promising strategy to treat metastatic cancers. Notwithstanding the excellent results in some tumors, the fraction of patients responding to immunotherapy remains low and combination of such pharmaceutical compounds with local therapy is considered necessary to increase the response. Combination with radiotherapy is interesting because ionizing radiation elicits an immune response, and checkpoint-blockers can inhibit the immune-suppressive tumor mechanisms that generally suppress the out-of-field effects of radiotherapy alone. Despite increasing the efficacy, still not all patients respond to this combination. We hypothesize that heavy ion therapy is more effective than X-rays in combination with immunotherapy. Indeed, particle therapy spares more lymphocytes thanks to the favorable dose-depth distribution, and may elicit immunogenic, molecular pathways more effectively than photons. We will show results of pre-clinical research which is aimed at understanding the molecular basis for improvement of particle therapy and its transfer to future medical applications in clinical protocols.

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Session Classi ication: Session I

Contribution ID: **194** Type: **Invited Talk**

Close Out

Wednesday, November 24, 2021 4:30 PM (20 minutes)

Session Classification: Session I