DS 1: Layer Properties: Electronic, Optical and Mechanical

Time: Monday 9:30–11:30 Location: H 0111

DS 1.1 Mon 9:30 H 0111

Tuning the probability of defect formation via substrate strains in Sr_2FeMoO_6 films — Waheed A. Adeagbo[1], •Martin Hoffmann[2], Arthur Ernst[2,3], Wolfram Hergert[1], Minnamari Saloaro[4], and Petriina Paturi[4] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [3]Max Planck Institute of Microstructure Physics, Halle, Germany — [4]Wihuri Physical Laboratory, Department of Physics and Astronomy, University of Turku, Finland

Since oxide materials like Sr_2FeMoO_6 are usually applied as thin films, we studied the effect of biaxial strain, resulting from a potential substrate, on the electronic and magnetic properties and, in particular, on the formation energy of point defects. From our first-principles calculations, we determined that the probability of forming point defects – like vacancies or substitutions – in Sr_2FeMoO_6 could be adjusted by choosing a proper substrate. For example, the amount of anti-site disorder and oxygen vacancies can be reduced with compressive strain to get purer Sr_2FeMoO_6 as needed for spintronic applications, while the formation of oxygen vacancies is more likely for tensile strain, which improves the functionality of Sr_2FeMoO_6 as basis material of solid oxide fuel cells. Hence, this degree of freedom might offer in general an additional possibility to tune the appearance of point defects besides e.g. experimental growth conditions like temperature or gas pressure.

DS 1.2 Mon 9:45 H 0111

Disorder Control in Crystalline $GeSb_2Te_4$ and its Impact on Characteristic Length Scales — •Matthias M. Dück[1], Tobias Schäfer[1], Marc Pohlmann[1], Carl-Friedrich Schön[1], Hannah Niehaus[1], and Matthias Wuttig[1,2] — [1]1. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Chalcogenides along the pseudobinary line between GeTe and Sb_2Te_3 (GST) are currently gaining much attention, since a number of interesting properties is observed in this material group, which contains phase-change materials, thermoelectrics, topological insulators and superconductors. Phase-change materials from the GST system have recently been reported to exhibit a disorder-induced metal-to-insulator transition, which is not linked to the transition from the metastable to the stable phase of this material. The MIT has been attributed to the ordering of stoichiometric vacancies, which leads to charge carrier delocalization. The current work is based on reports of a correlation between vacancy layer formation in textured films and their electronic transport properties. A systematic study of low temperature transport in combination with highly textured GST thin films provides further insights in the mechanisms of disorder induced charge carrier localization. In this talk, the relationship between characteristic length scales for atomic arrangement as well as electronic transport in the GST124 system will be elucidated. A comparative analysis of the results reveals the importance of vacancy ordering in this system, as well as the insignificance of grain boundaries for the material's properties.

DS 1.3 Mon 10:00 H 0111

2D protective films for lithium and sodium metal anodes — Hongzhen Tian[1], Zhi W. Seh[2], Kai Yan[2], Zhongheng Fu[1], Peng Tang[1], Yingying Lu[3], Ruifeng Zhang[1], •Dominik Legut[4], Yi Cui[5], and Qianfan Zhang[1] — [1]School of Materials Science and Engineering,Beihang University, Beijing 100191, China — [2]Institute of Materials Research and Engineering Agency for Science, Technology and Research, Innovis, Singapore 138634, Singapore — [3]State Key Laboratory of Chemical Engineering College of Chemical and Biological Engineering Zhejiang University Hangzhou 310027, China — [4]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [5]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA

Rechargeable batteries based on lithium (sodium) metal anodes have been attracting increasing attention due to their high capacity and energy density, but exhibit drawbacks, such as low Coulombic efficiency and dendrites growth. Lay- ered materials have been used experimentally as protective films (PFs) to address these issues. Here we use first-principles calculations to determine the properties and feasibility of various 2D layered PFs.It is found that the introduction of defect, the increase in bond length, and the proximity effect by metal can accelerate the transfer of Li^+ (Na^+) ion and improve the ionic conductivity, but all of them make negative influences on the stiffness of materials. [1] H. Tian et al, Advan. Ene. Mat. **7**, 1602528 (2017).
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DS 1.4 Mon 10:15 H 0111

Development of mirror coatings for gravitational wave detectors — •Lukas Terkowski[1], Jessica Steinlechner[1,2], Daniel Axmann[1], Jim Hough[2], Iain Martin[2], Sheila Rowan[2], and Roman Schnabel[1] — [1]Institut für Laser-Physik, Universität Hamburg, Luruper Chaussee 149, Gebäude 69, 22761 Hamburg, Germany — [2]SUPA, School of Physics and Astronomy, University of Glasgow, Glasgow, G12 8QQ, Scotland

Gravitational waves are ripples in space caused by massive, accelerated objects in space. They were predicted by Einstein more than 100 years ago and first measured in 2015. When reaching their design sensitivity, current gravitational-wave detectors - as well as all planned, future detectors - will be limited, at their most sensitive frequencies, by thermal noise from the highly-reflective mirror coatings.

To detect more, weaker gravitational waves from a wider range of astrophysical sources, it is necessary to develop new coating materials. Besides low thermal noise, there are also strong requirements on the optical absorption and optical scattering of the coatings, which have to be available in large sizes.

Due to low thermal noise, amorphous silicon seems to be a promising solution for a coating material. However, the optical absorption of commercially available amorphous silicon is currently far higher than the requirement. In this talk we will present our work on improving the optical properties of amorphous silicon by optimizing deposition parameters, to make future gravitational-wave detectors more sensitive.

DS 1.5 Mon 10:30 H 0111

Quantitative AM-FM Mode for Fast, Versatile Imaging of Nanoscale Elastic Modulus — •Florian Johann, Roger Proksch, Marta Kocun, and Ted Limpoco — Oxford Instruments (Asylum Research), Santa Barbara, USA

Nanoscale information on mechanical properties is critical for many advanced materials and nanotechnology applications. Atomic Force Microscopy (AFM) techniques for probing mechanical properties of samples in the nanometer range have emerged over the past decades.

Amplitude-modulated AFM (AM-AFM), also known as tapping mode, is a proven, reliable and gentle imaging method with widespread applications. Previously, the contrast in AM-AFM has been difficult to quantify. Here, we introduce AM-FM imaging, which combines the features and benefits of normal tapping mode with quantitative and high sensitivity of frequency modulated (FM) mode. Briefly, the topographic feedback operates in AM mode while the second resonant mode drive frequency is adjusted on resonance. With this approach, frequency feedback and topographic feedback are decoupled, allowing much more stable, robust operation. The FM image returns a quantitative value of the frequency shift that depends on the sample stiffness and can be applied to a variety of physical models.

DS 1.6 Mon 10:45 H 0111

Layer specific observation of the slow thermal equilibration in ultrathin metallicnanolayers by femtosecond x-ray diffraction — Jan-Etienne Pudell[1], Alexey Maznev[2], Marc Herzog[1], Matthias Kronseder[3], Christian Back[3], Gregory Malinowski[4], •Alexander von Reppert[1], and Matias Bargheer[1,5] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Department of Chemistry, Massachusetts Institute of Technology, Massachusetts, USA — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [4]Institut Jean Lamour (UMR CNRS 7198), Université Lorraine, Nancy, France — [5]Helmholtz-Zentrum Berlin, Berlin, Germany

We study the ultrafast response of nanometric layers of Gold (Au) on Nickel (Ni) upon optical excitation with femtosecond laser pulses by ultrafast x-ray diffraction (UXRD). We show the experimental results

obtained by exciting a 12 nm Ni film through a 5 nm Au film by 800 nm pulses with about 50 fs pulse duration. Although the pump pulse impinges on Au, the initially deposited energy is essentially transferred to the Ni lattice due to its much larger electron phonon-coupling constant. The most surprising result is the very slow heat transport from Ni into the Au lattice. The Au lattice temperature reaches its maximum only after 80 ps, although bulk heat conductivity estimates would predict less than 1 ps to equilibrate the temperatures of the two ultrathin metal layers. UXRD thus represents a formidable experimental probe to support theoretical developments in nanoscale thermal transport.

DS 1.7 Mon 11:00 H 0111

Revealing Charge Redistribution at Hybrid Interfaces by DRS — •Tino Meisel[1], Marcel Gawek[1], Mino Sparenberg[1], Sergey Sadofev[1], Oliver Benson[1], Emil J. W. List-Kratochvil[1,2], and Sylke Blumstengel[1,2] — [1]Institute of Physics, Humboldt University Berlin — [2]Institute of Chemistry, Humboldt University Berlin

Hybrid inorganic/organic systems (HIOS) combining functional conjugated molecules and inorganic semiconductors are promising candidates for opto-electronic devices such as photovoltaic cells and light emitting diodes. For these applications understanding of the interfacial electronic structure plays a key role. In this work we present differential reflectance spectroscopy (DRS) as a novel experimental tool to reveal ground state charge transfer at hybrid interfaces. As prototypical HIOS conjugated molecules (ladder-type quaterphenyl (L4P), NTCDA, F6TCNNQ) were deposited on top of epitaxial ZnO via molecular beam deposition and DRS was conducted in real time in the course of the organic layer growth. Two types of HIOS interfaces will be discussed: (i) HIOS with negligible interfacial charge transfer (L4P/ZnO). In this case the DR spectra can simply be modelled using the dielectric functions of the individual layers. (ii) HIOS with ground state charge transfer at the interface (F6TCNNQ/ZnO, NTCDA/ZnO). Here, the dielectric function of ZnO is significantly altered by the interaction with the molecules which causes a characteristic fingerprint in the DR spectra. DRS is thus viable tool to uncover interfacial charge carrier redistribution at HIOS interfaces.

DS 1.8 Mon 11:15 H 0111

Non-degenerate valleys in transition metal layered WS_2 — •Omar Messaoudi[1,2], Julen Ibañez-Azpiroz[2], and Samir Lounis[2] — [1]Université Mouloud Mammeri de Tizi Ouzou, Tizi Ouzou, Algeria — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

We present a comparative first principles investigation of the electronic properties of monolayer WS2 coated with an overlayer of a transition metal (Fe, Co, Mn). Fe outstands as the most prominent candidate where our ab initio calculations reveal that the system is a half-metallic ferromagnet with a gap of 1 eV for the majority spin channel. Furthermore, the combined effect of time-reversal symmetry breaking, due to the magnetic Fe overlayer, and the large spin-orbit coupling induced by W gives rise to non-degenerate K and K$*$ valleys. This has a tremendous impact on the excited state properties induced by externally applied circularly polarized light. Our analysis demonstrates that the latter induces a singular hot spot structure of the transition probability around the K and K$*$ valleys for right and left circular polarization, respectively. We trace back the emergence of this remarkable effect to the strong momentum dependent spin-noncollinearity of the valence band involved. As a main consequence, a strong valley-selective magnetic circular dichroism is obtained, making this system a prime candidate for spintronics and photonics applications.