DS 13: Poster

Time: Thursday 18:00–20:00 Location: P1

DS 13.1 Thu 18:00 P1

Establishing Circular Dichroism Spectroscopy as predictor for CISS in molecular thin films — •Franziska Schölzel[1,3], Dominik Hornig[2,3], Lokesh Rasabathina[1], Olav Hellwig[1,3], Michael Mehring[2,3], and Georgeta Salvan[1,3] — [1]TU Chemnitz, Institute of Physics, 09126 Chemnitz, Germany — [2]TU Chemnitz, Institute for Chemistry, 09111 Chemnitz, Germany — [3]TU Chemnitz, Research Center for Materials, Architectures and Integration of Nanomembranes, 09126 Chemnitz, Germany

Circular Dichroism Spectroscopy which utilizes the differential absorption of left and right circularly polarized light to distinguish between the enantiomers of a chiral molecule. Previously it has been shown that the method is able to predict the strength of the chirality induced spin selectivity (CISS) effect [1]. Although many studies show that CISS relies on the interface between a chiral molecule and a magnetic substrate, CD spectroscopy is mainly used for the analysis of molecules in solution [1]. Therefore, it is crucial to develop a method for the interpretation of CD exhibited by molecular thin films.

In this study we present a homebuilt setup to implement the analysis of thin films systems into the Jasco J-1500 CD spectrophotometer. Furthermore, we propose a way to overcome artefacts that may be caused by optical anisotropy of the film and the substrate [2].

[1] Chem. Rev. 124, 4, 1950-1991 (2024) [2] J. Am. Chem. Soc. 143, 21519-21531 (2021)

DS 13.2 Thu 18:00 P1

Wannier description using CP2K — •Nisarg Trivedi, Maximilian F. X. Dorfner, and Frank Ortmann — School of Natural Sciences, Technische Universität München

Wannier functions provide an ideal basis for simulating quantum transport using Model Hamiltonians (i.e., tight binding models). Most Wannier generation tools use a plane-wave basis to expand the Wannier functions. However, using a gaussian basis to expand such functions can make simulations more efficient by using the sparsity of the matrices. Here, we present a procedure to obtain moderately localized Wannier functions on an atom-centered gaussian basis. Interfaced with the CP2K software, the method uses the Kohn-Sham Hamiltonian and Overlap matrices obtained from DFT simulation in the same atom-centered gaussian basis to obtain the Bloch states and then transform them into Wannier functions. We present the results of the application of this method on different polymers, which show excellent reproduction of band structure using a simple tight binding model based on the respective Wannier functions for all studied polymers.

DS 13.3 Thu 18:00 P1

Geometry and electronics of helical nanostructures — •Faezeh Shabani[1], Sibylle Gemming[1], Florian Günther[2], Jeffrey Kelling[1], Hadis Ghodrati Saeini[1], Christoph Tegenkamp[1], Thi Ngoc Ha Nguyen[1], and Georg Kuenze[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil — [3]Universität Leipzig, Leipzig, Germany

Helical nanostructures are intriguing systems where geometry and chirality drive unique electronic phenomena, including the chiral-induced spin selectivity (CISS) effect. This interplay enables efficient spin polarization in electron transport, offering exciting prospects for spintronic applications. In this study, the electronic band structure of helical nanostructures is explored, highlighting how their geometry influences transport as well as spin-dependent properties. These insights will inspire further investigations into biological helices, such as peptides and proteins, which share similar structural motifs and could broaden our understanding of spin polarization in natural systems. This work is part of TRR 386 HYPMOL, funded by DFG. (www.hypmol.net)

DS 13.4 Thu 18:00 P1

local charge transport properties of n-type organic semiconductor films based on T2-(NDI-T2)2 — •Zihao Liu[1], Hajar Komekoz[1], Nisarg Trivedi[2], Dietrich R. T. Zahn[1], Michael Sommer[1], Frank Ortmann[2], and Georgeta Salvan[1] — [1]Fakultät für Naturwissenschaften, Semiconductor Physics group, Technische Universität Chemnitz — [2]TUM School of Natural Sciences,Technische Universität München

Due to the advantages of organic semiconductor thin films, such as weak spin-orbit coupling and low spin scattering, organic materials have emerged as a strong alternative to traditional metallic spacer layers in the field of spin valve devices with vast potential for future spintronic applications. This study investigates conjugated organic semiconductor materials, specifically T2-(NDI-T2)2, and its related compounds with different side chain lengths focusing on their electrical properties on the micrometer and nanometer scales. High-quality organic semiconductor thin films were fabricated on gold substrates by spin coating. The dielectric function ϵ and the film thicknesses were determined by spectroscopic ellipsometry. Kelvin Probe Force Microscopy (KPFM) and conductive atomic force microscopy (c-AFM) were employed to analyze the local charge transport properties of the films systematically. The findings provide crucial insights into the influence of molecular orientation on conductivity and charge carrier mobility providing a solid foundation for further understanding and application of organic semiconductor materials

DS 13.5 Thu 18:00 P1

A graph-theoretical approach to spin-polarised quantum walks in chiral environment — •Saba Arshad[1], Sibylle Gemming[1], and Shahid Iqbal[2] — [1]TU Chemnitz, Chemnitz, Germany — [2]NUST, Islamabad, Pakistan

Exploring the model where a particle or system of particles moves between neighboring nodes couple with autonomous spins on the edges, leading to the propagation of entanglement. The work highlights how entanglement, along with spin oscillations and relaxation dynamics, offers significant advantages while transmitting directed quantum information through the quantum walks, providing faster quantum computations. This approach establishes a connection between spin dynamics and quantum computation, with potential applications in cryptography, quantum key distribution, super-dense coding, teleportation, and quantum computing, leveraging entangled states for secure and efficient information processing.

DS 13.6 Thu 18:00 P1

Self-Assembly Kinetics of Polyalanine α-helix Monolayers: Insights from Coarse-Grained Molecular Dynamics Simulations — •Hadis Ghodrati Saeini[1], Thi Ngoc Ha Nguyen[1], Faezeh Shabani[1], Olav Hellwig[1,2], Christoph Tegenkamp[1], Sibylle Gemming[1], Florian Günther[3], and Jeffrey Kelling[1,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute for Ion Beam Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo (USP), São Carlos, Brazil — [4]Institute for Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany

Helical molecules, such as polyalanine α-helices, are promising candidates for spintronic applications due to their strong spin-filtering ability via the Chiral-Induced Spin Selectivity (CISS) effect. Understanding their intermolecular interactions and collective behavior is essential for harnessing their properties in practical applications. This study employs molecular dynamics simulations with coarse-grained molecular potentials to explore the kinetics of monolayer self-assembly by deposition from solution onto a smooth van der Waals substrate.

Simulations conducted at room temperature reveal key aspects of molecular relaxation, structural organization, and dynamical timescales. These insights enhance our understanding of the self-assembly mechanisms and stability of polyalanine monolayers, supporting their development for advanced spintronic technologies.

DS 13.7 Thu 18:00 P1

Simulation of self-assembled polyalanine α-helices films: Development and application of an empirical potential — Kevin Preis[1], Hadis Ghodrati Saeini[1], Christoph Tegenkamp[1], Sibylle Gemming[1], Jeffrey Kelling[2], and •Florian Günther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]São Paulo State University, Rio Claro, Brazil

Polypeptide molecules have been discussed as potential candidates for electronic spin-filters because of the so-called chiral-induced spin se-

lectivity. For this reason, tremendous effort is invested to characterize the structural and electrical properties of self-assembled monolayers (SAMs) of peptide helices, e.g. polyalanine (PA) α-helices. In our work, we aim at characterizing the intermolecular interactions that govern the formation of PA-SAM films. For this, we elaborated an empirical potential that models the interaction of two isolated helices using the density functional based tight-binding method. With these potentials, energetically most favored arrangements in SAM films were simulated via a Monte-Carlo approach using the simulated annealing and the Metropolis algorithm. Statistically analyzing the relative positioning of adjacent molecules, we are able to classify the degree of frustration in SAM films. For enantiopure systems, we found that a frustration-free arrangement is possible yielding a perfect hexagonal lattice. For mixtures of different chiralities, parallel aligned domains of differently handed helices were obtained. Both of these observations are in great agreement to experimental works.

DS 13.8 Thu 18:00 P1

Thin films of atomically precise chiral bismuth oxido nanoclusters — •Dominik Hornig[1], Rico Thomas[1], Annika Morgenstern[2], Franziska Schölzel[2], Thi Ngoc Ha Nguyen[2], Christoph Tegenkamp[2], Georgeta Salvan[2], and Michael Mehring[1] — [1]TU Chemnitz, Institute of Chemistry, Germany — [2]TU Chemnitz, Institute of Physics, Germany

The adsorption of chiral molecules on metallic surfaces induces electron spin polarization at the interface, enabling novel applications in chiral opto-spintronics. This effect, known as chiral-induced spin selectivity (CISS), strongly depends on the binding and ordering of the species on surfaces.[1] In our studies, we investigate the adsorption behavior of chiral bismuth oxido nanoclusters (BiO-NCs) on gold (Au) surfaces. The chiral BiO-NCs represent monodisperse nanoclusters which can be modulated by an exchangeable ligand shell. This has been demonstrated for the stable $[Bi_{38}O_{45}]$ cluster architecture and enables targeted modification of the BiO-NC with regard to optical properties.[2,3] By functionalizing BiO-NCs with amino acids such as Boc-L-methionine and Boc-L-phenylalanine, the chiral nanoclusters $[Bi_{38}O_{45}(\text{Boc-L-Met-O})_{24}]$ or $[Bi_{38}O_{45}(\text{Boc-L-Phe-O})_{24}]$ were synthesized. Furthermore, tuning of physical properties is possible by doping these atomically precise nanoclusters with other metals. Here we present the preparation of thin films of atomically precise chiral BiO-NCs and results of ellipsometry, UV-Vis, STM and STS measurements. [1] Nat. Rev. Chem. 2019, 3, 250-260. [2] Langmuir 2024, 40, 16320-16329.[3] Nanomaterials 2022, 12, 1815.

DS 13.9 Thu 18:00 P1

Twist angle dependent proximity induced spin-orbit-coupling in graphene/NbSe2 heterostructures — •Thomas Naimer[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Pavol Jozef Safarik University in Kosice, 04001 Kosice, Slovakia

We investigate the effect of the twist angle on the proximity spin-orbit coupling (SOC) in graphene/niobium diselenide (Gr/NbSe2) heterostructures from first principles. The low energy Dirac cones of several different commensurate twisted supercells are fitted to a model Hamiltonian, allowing us to analyze the twist-angle dependency of the SOC in detail. This reveals the possibility to triple the Rashba SOC, when going from 0° to 30° twist angle. Furthermore, at a critical twist angle of 23° the in-plane spin structure acquires a significant radial component, enabling collinear charge-to-spin conversion. Analyzing the Dirac cone with respect to allowed Umklapp processes and orbital decomposition shines light on the observed twist angle dependencies. In addition we evaluate the potential for (collinear and perpendicular) charge-to-spin conversion in such heterostructures within linear response theory. All authors acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH. T. N. and J. F. were also supported by the European Union Horizon 2020 Research and Innovation Program 881603 (Graphene Flagship). M.G. acknowledges additional financial support provided by the Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114 and Slovak Academy of Sciences project IMPULZ IM-2021-42.

DS 13.10 Thu 18:00 P1

Wet-Chemical Transfer and Post Characterization of Hexagonal Boron Nitride Grown on Ge(001)/Si Substrates — •Monika Choudhary[1], Max Franck[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP-Leibniz-Institut für Innovative Mikroelektronik, Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

This study presents a poly (methyl methacrylate) (PMMA) assisted transfer process for hexagonal boron nitride (hBN) epitaxially grown on Ge(001)/Si substrates via chemical vapor deposition using borazine at 900-980°C. The transfer involves sequential etching of Si at 95°C in KOH solution [1] and of Ge in NH4OH, H2O2, and H2O solution (1/1/5) at 75°C [2]. The PMMA/hBN is then transferred onto SiO2/Si and TiN/Si substrates, confirmed by optical microscopy, Raman and X-ray photoelectron spectroscopy analyses. Furthermore, metal-insulator-metal devices are fabricated by gold deposition on hBN/TiN, yielding a resistivity of 5.1e-10 ohm*cm and a dielectric constant of 2.4, as determined by current-voltage and capacitance-voltage measurements. Additionally, hBN/graphene/hBN heterostructures are fabricated and characterized using optical microscopy and Raman analyses. Hall bar devices are then created by defining structures on the hBN/graphene/hBN stack using photolithography and reactive ion etching.

[1] P. Pal, et al. Micro and Nano Systems Letters 9 (2021):4. [2] S. Sioncke, et al. Solid State Phenomena 145-146 (2009):203-206.

DS 13.11 Thu 18:00 P1

Tuning the electronic structure of MoSe2 through molecular adsorbates — •Carolin Sabrina Schüle, Joschua Büble, and Heiko Peisert — Institut für Physikalische und Theoretische Chemie Universität Tübingen, Deutschland

Layered transition metal dichalcogenides have emerged as a promising alternative to conventional semiconductor materials. The electronic properties of TMDCs can be tuned by the adsorption of molecules, including weakly interacting, physisorbed carbon molecules. As example, a quenching of the low-temperature defect photoluminescence of MoS2 was observed after adsorption of metal-phthalocyanines, depending strongly on the central metal atom of the phthalocyanine.1 We studied interface properties of phthalocyanines (CoPc and CoPcF16) on MoSe2 and p-doped MoSe2 as example for comparably weakly interacting molecules, and compare them to HATCN - a strong electron acceptor. For the cobalt phthalocyanines, the exchange of the metal centre has only a small effect on the position of the highest occupied molecular orbital (HOMO), whereas fluorination of the molecular backbone lowers the HOMO considerably. The formation of dipols, interface states, as well as a band bending in the MoSe2 bulk substrates was observed, depending on the molecule under consideration. (1) DOI: 10.1021/jacs.1c07795.

DS 13.12 Thu 18:00 P1

Synthesis of MoS_2 films for electronic and optoelectronic device applications — •Axel Printschler, Md Tarik Hossain, Julian Picker, Christof Neumann, and Andrey Turchanin — Friedrich-Schiller-Universität Jena, Institute of Physical Chemistry, Jena, Deutschland

Transition metal dichalcogenides (TMDs) are a class of 2D materials that have exceptional promise for a wide range of electronic and optoelectronic applications. In particular, TMD-based field-effect transistors (FETs) are continually in the focus of research because of their potential to overcome the limitations of traditional silicon-based devices. To efficiently fabricate FETs based on TMD monolayers, it is crucial to synthesize continues mono- or few layers of these materials on wafer scale and/or enable their growth at a predefined position on the wafer. In this study, we compare different methods for bottom-up synthesis of MoS_2 monolayers and thin films and characterize their properties for device applications. To this end, we employ CVD growth from solid and liquid state precursors as well as MOCVD growth using gaseous precursors. The synthesized films are characterized using complementary spectroscopy and microscopy techniques including optical and atomic force microscopy (AFM), X-ray photoelectron, Raman and photoluminescence (PL) spectroscopy, which is further complemented by electrical and optoelectrical measurements of the microfabricated FET devices.

DS 13.13 Thu 18:00 P1

Conventional and nanoscale NMR investigation of NbSe2 for various temperatures, magnetic field strengths and orientations — •Mokessh Kannah Ciwan[1], Marcel Martin[1], Jakob Nachtigal[1], Yejin Lee[4], Nicola Poccia[2,3], Uri Vool[4], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]Department of Physics, University of Naples

Federico II, Naples, Italy — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Niobium diselenide (NbSe2) is a transition metal dichalcogenide (TMD) that has attracted particular interest for decades due to the coexistence/competition of charge density waves (CDW) and the superconducting state in the bulk crystal. To this end, nuclear magnetic resonance (NMR) can be used to measure relaxation times and shifts in the resonance frequency, which reveal how the charge carriers in these phases interact with the nuclei of the host material.

Using conventional NMR, we investigate the electronic behaviour of bulk NbSe2 over a wide range of magnetic field amplitudes and orientations as well as temperatures down to the CDW phase. Additionally, we are working towards nanoscale NMR using nitrogen vacancy (NV) centers in diamond as quantum sensors. This method allows NMR measurements on um-scale exfoliated flake down to the monolayer. In this direction we have already achieved first promising results. Findings from both bulk and flake measurements will be presented.

DS 13.14 Thu 18:00 P1

A Hybrid Organic-hBN Platform for Quantum Sensing — •Xuan-Kai Zhou, Yan-Tung Kong, Ruo-Ming Peng, and Jörg Wrachtrup — Universität Stuttgart, 3. Physikalisches Institut, Allmandring 13, Stuttgart, Deutschland

Optically activated molecular spin qubits are promising candidates for quantum sensing applications due to their customizable molecular design, enabling biocompatibility and close proximity to target environments. However, organic molecules under ambient conditions often suffer from weak emission signals, instability, and degradation caused by solvent evaporation, air exposure, and low resistance to photobleaching during measurements. In this work, we address these challenges by encapsulating organic molecules within two-dimensional hexagonal boron nitride (2D-hBN) rather than diluting them in conventional host organic polymers such as p-terphenyl. This hybrid organic-2D material heterostructure stabilizes the fluorescence of organic molecules, potentially enhancing the performance of optically detected magnetic resonance (ODMR) measurements. Furthermore, this innovative encapsulation method integrates physical chemistry into 2D materials approaching the monolayer limit, significantly advancing sensing capabilities, including surface-sensitive techniques and biocompatible detection strategies.

DS 13.15 Thu 18:00 P1

Towards infrared photodetection with an ultra-low carrier density moiré superconductor — Giorgio Di Battista[1], •Leon G. Schubert[1], Kin Chung Fong[2,3], Andrés Díez-Carlón[1], Kenji Watanabe[4], Takashi Taniguchi[5], and Dmitri K. Efetov[1,6] — [1]Fakultät für Physik, LMU — [2]Department of Physics, Harvard University — [3]Quantum Engineering and Computing Group, Raytheon BBN Technologies — [4]Research Center for Functional Materials, NIMS, Tsukuba — [5]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba — [6]Munich Center for Quantum Science and Technology (MCQST)

Single-photon detectors (SPDs) offer remarkable capabilities for highly-sensitive detection of electromagnetic radiation. To achieve high performance, state-of-the-art SPDs rely on the photon-induced breaking of Cooper pairs in superconductors (SCs). However, extending SPD capabilities to lower photon energies requires novel SC materials with significantly lower charge carrier densities which offer a larger relative perturbation of the SC state. The moiré superconductor magic-angle twisted bilayer graphene (MATBG) holds great promise with its unprecedentedly low carrier density of $\sim 10^{11}\mathrm{cm}^{-2}$ which is ~ 5 orders of magnitude lower than conventional SCs. We demonstrate a proof-of-principle experiment to detect single near-infrared photons by voltage biasing a MATBG device near its SC phase transition. Our work offers insights on the MATBG-photon interaction and opens new opportunities for developing novel quantum sensors with the potential for single photon detection in the terahertz spectrum.

DS 13.16 Thu 18:00 P1

Qauntum anomalous Hall effect in Cr-doped BST — •Edoardo Tosi[1,2], Gertjan Lippertz[1], Anjana Uday[1], Bibek Bhujel[1], Alexey Taskin[1], Marco Moretti[2], and Yoichi Ando[1] — [1]University of Cologne — [2]Polytechnic University of Milan

The quantum anomalous Hall (QAH) effect in a magnetic topological insulator (TI) represents a new state of matter originating from the interplay between topology and magnetism. The defining characteristics of the QAH ground state are the quantized Hall resistivity and vanishing longitudinal resistivity in the absence of an external magnetic field. Manipulating the QAH state is of great importance in both the understanding of topological quantum physics and the implementation of dissipationless electronics.

To observe the QAH effect, fabrications of thin-film devices are required which allows for tuning the Fermi level across the Dirac point. It is necessary to improve growth conditions for the ternary compound (Bi1-xSbx)2Te3 such that the composition between n-type Bi2Te3 and p-type Sb2Te3 can be almost perfectly compensated. Decreasing the thickness of the MBE grown films, reduces the bulk-to-surface ratio and leads to TI samples where the surface transport is dominating. Doping ultrathin films with Cr allows to obtain the ferromagnetic state, which opens a gap in the surface states, leading to the QAH effect at low temperatures.

In this contribution we report our efforts to realize the QAH effect in the magnetic topological insulator Cr-doped (Bi,Sb)2Te3 (CBST) grown by molecular beam epitaxy (MBE) on an InP substrate.

DS 13.17 Thu 18:00 P1

VO2 oscillator with advanced neuron-like feature originating from blinking filament — •Zhong Wang, Kajal Tiwari, Yishen Xie, Jae-Chun Jeon, Ke Xiao, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle(Saale), Germany

The insulator-metal-transition of VO2 gives rise to the electric oscillation that has extensive applications in neuromorphic computing[1]. Although the oscillation feature is typically stable and deterministic, advanced neuromorphic applications require more complex and adaptive device properties[2]. Here we discover the neuron-like bursting with the non-deterministic separation time in the VO2 thin film-based device, which is only detectable in a narrow temperature range below transition. This feature of VO2 indicates the dynamical process beyond ordinary insulator-metal-transition and capacitive charging. By scanning near-field optical microscopy and modelling, we identify the flipping filament formation in multiple positions as the physical origin of the complex feature observed. Our work unveils the mechanism underlying VO2 oscillator that could assist future device design for neuromorphic computing.

[1] P. Schofield et al., Advanced Materials 35, 2205294 (2023).
[2] S. Kumar et al., Nature Reviews Materials 7, 575 (2022).

DS 13.18 Thu 18:00 P1

Advanced modeling of X-ray reflectivity for metallic multilayer systems with GenX 3 — •Rico Ehrler[1,2] and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Research Center MAIN, D-09126 Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany

X-ray reflectivity (XRR) is a versatile, nondestructive technique for probing thin film systems at grazing incidence, offering insights into layer thickness, roughness, and density. However, due to the inherent phase problem in X-ray techniques, extracting these parameters from the XRR data requires careful sample modeling. Especially for metallic multilayers with a complex microstructure, creating a well parametrized model may be challenging. We explore different modeling approaches using the open-source software "GenX 3"[1] on the example of sputter deposited, magnetic Co/Pt multilayer systems. A simplified model without the complex multilayer structure is found to fit the data surprisingly well, when limiting the XRR to a reasonable range. We then add the actual multilayer, modeled with a damped, periodic function following a graded-interface approach to account for the complex microstructure.[2] Finally, real space transmission electron microscopy (TEM) images are used to motivate and validate the models.

[1] A. Glavic and M. Björck, J. Appl. Cryst., **55**, 1063-1071 (2022)
[2] V. Munteanu et al., J. Appl. Cryst., **57**, 456-469 (2024)

DS 13.19 Thu 18:00 P1

In-Situ XAS study of ZnO and Mn-ZnO thin films — •Sulaiman Al Salem[1,2], Sreeju Sreekantan Nair Lalithambika1[2], Shagun Thakur[3], Simone Techert[1,2,3], and Christian Jooss[3] — [1]Institute of X-ray Physics, University of Göttingen, 37077 Germany — [2]Structural Dynamics in Chemical Systems, Deutsches Elektronen-Synchrotron, DESY, Notkestrasse 85, D-22607, Hamburg, Germany — [3]Institute of Materials Physics, University of Göttingen, 37077 Germany

High-performance catalysts with low overpotential for oxygen evolution reaction (OER) are critical for green energy transition. Transition metal-doped ZnO thin films make it a promising catalyst for efficient OER. Understanding the electronic properties of such materials in a catalytically relevant environment is crucial for tailoring and tuning these materials for OER applications. X-ray Absorption Spectroscopy (XAS) is a powerful spectroscopic technique that is element-selective and environment-sensitive. We present an investigation into the electronic structure of Zinc Oxide (ZnO) and Mn-doped thin films using XAS at the Oxygen K-edge as well as the Zn and Mn L-edges. The XAS spectra, which serve as the basis for further investigation upon Mn-doping, show the characteristic peaks of the elements present in the films. Besides, soft x-ray XAS spectra at in-situ ZnO and Mn-doped ZnO - water interface conditions were measured further to study the electronic structure at catalytically relevant conditions.

DS 13.20 Thu 18:00 P1

Martensitic Transformation in Ultrathin Layered Stacks of $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$ — •Nancy Töws, Pascal Strathkötter, Roland Schubert, Inga Ennen, Judith Bünte, Laila Bondzio, Dario Stierl, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld, Germany

Magnetic shape memory alloys, such as various Heusler alloys, have been extensively studied over the past decade for their potential in magnetocaloric applications. In the realm of thin-film technology, stacking different Heusler alloys in layered systems offers a microstructural design framework initiated through the interaction of strain fields during the martensitic transformation of the stack*s individual components*.

Here, we present results on the stacking of two well-known FeNi alloys, $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$, and the resulting physical properties. We report on investigations conducted using structural, magnetic, and thermal methods, alongside findings on the progression of martensitic and austenitic transformations within these distinct layered systems.

*Reference: Ramermann et al., *Nano Scaled Checkerboards: A Long-Range Ordering in NiCoMnAl Magnetic Shape Memory Alloy Thin Films with Martensitic Intercalations,* Appl. Sci. 2022, 12(3), 1748; https://doi.org/10.3390/app12031748.

DS 13.21 Thu 18:00 P1

Structural and electronical investigation of the Electrode/MoS2 interface by electron microscopy and photoemission — •Eric Juriatti, Christoph Späth, Heiko Peisert, and Marcus Scheele — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Tübingen, Germany

In search for new semiconducting devices the group of transition-metal dichalcogenides (TMDCs) like molybdenum disulfide (MoS2) is of increasing scientific interest. The exceptionally unique electronic properties, including the tunability of the band gap by exfoliation, of these layered semiconductors allow further miniaturization of devices like photodetectors, which are promising candidates to fulfill Moore*s law in future applications.

The successful manufacturing of astonishingly fast and responsive TMDC photodetectors contacted by gold electrodes was recently demonstrated. However, the influence of the electrodes on the TMDC/metal interface properties, which would supposedly also affect charge carrier transport in devices, has not been studied in detail so far.

In this study, different metals which are typical electrode materials were deposited as thin films on clean MoS2 bulk crystals to mimic the resulting TMDC/Metal interface. The resulting heterostructure was investigated by X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS). In addition, scanning electron microscopy (SEM) was performed to study the growth of the metals on the TMDC surface.

DS 13.22 Thu 18:00 P1

Transition metal oxide doped ZnO films for electro-synthesis — •Shagun Thakur, Pia Henning, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Germany

Understanding the crystal structure and morphology is crucial for investigating the electrocatalytic activity of inorganic materials. Zinc oxide doped with transition metal oxides are interesting candidates for electro-conversions owing to their unique reactivity. The ZnO crystal exhibits different polarity and surface stability in different crystallographic directions [1][2]. With this aim of producing well-defined ZnO films, we utilized the advancements of thin film technology.

Sputtering is used for growing epitaxial undoped and Mn-doped ZnO thin films with temperature and oxygen control. We will also use pulsed laser deposition which is modified by attaching molecular beam sources to prepare such surfaces with precise fine-doped elements and stoichiometry control. These films will be later compared.

This work presents our ongoing studies on transition metal-doped ZnO thin films, focusing on magnetic dopants and their impact on catalytic activity via sputtering and hybrid PLD systems.

[1] C.-H.P. Sung-Ho Na, First-Principles Study of the Surface of Wurtzite ZnO and ZnS - Implications for Nanostructure Formation, The Journal of the Korean Physical Society, 54 (2009) 5

[2] S. Akhter, K. Lui, H.H. Kung, Comparison of the chemical properties of the zinc-polar, the oxygen-polar, and the nonpolar surfaces of zinc oxide, The Journal of Physical Chemistry, 89 (1985) 1958-1964

DS 13.23 Thu 18:00 P1

Tuning high-T_C ferromagnetism and perpendicular magnetic anisotropy in van der Waals magnet $Cr_{1+\delta}Te_2$ — •Laura Pflügl, Pia Henning, Anna Tschesche, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In recent years, chromium tellurides ($Cr_{1+\delta}Te_2$) have gained significant interest due to their promising characteristics, such as ferromagnetic ground states with tunable transition temperatures and perpendicular magnetic anisotropy (PMA) which open up various possible applications in spintronics [1]. However, the fabrication of high-quality stochiometric and epitaxial $Cr_{1+\delta}Te_2$ thin films is difficult and calls for advanced synthesis techniques. Using a hybrid setup combining pulsed laser deposition for Cr and a molecular beam source for Te, we deposited $Cr_{1+\delta}Te_2$ thin films with precise stoichiometry control [2]. Changes of the magnetism were previously reported in $Cr_{1+\delta}Te_2$ due to extreme air-sensitivity and nonself-limited oxidation [3]. Since our films are epitaxially stabilized on a substrate, they are free from defect introduction and offer air stability by forming a passive surface oxide layer. We will address the ongoing challenges during the growth of this material and put forward effective tuning by varying deposition control parameters.

[1] Y. Fujisawa et al., Phys. Rev. Mater., 4 (2020) 114001.

[2] A. Tschesche, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

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DS 13.24 Thu 18:00 P1

Investigating interfacial mechanisms and switching behavior in GST-124/Sb_2Te_3 superlattices using Atom Probe Tomography — •Athanasia Piperidou[1], Jan Köttgen[1], Lucas Bothe[2], Lukas Conrads[1], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Chalcogenide-based phase-change materials like $GeSb_2Te_4$ (GST) are crucial for non-volatile storage technologies due to their rapid and reliable switching. Reducing the energy required for transitions between amorphous and crystalline states can improve device performance significantly, as demonstrated in phase-change memories using superlattices (SLs). Here we investigate the switching behavior of MBE-grown 60nm GST-124/Sb_2Te_3 SLs. Using a pulsed laser, we induce amorphization and recrystallization processes. Atom Probe Tomography (APT) is used to compare the structural and chemical characteristics of interfaces in recrystallized and as-deposited regions. APT's three-dimensional, near-atomic resolution reveals changes in morphology and element distribution, shedding light on the mechanisms driving switching. Our results show that the SL structure enhances switching efficiency through unique interfacial mechanisms, offering insights for the design of next-generation memory devices.

DS 13.25 Thu 18:00 P1

Deposition of Medium-Entropy Telluride Thin Films via Hybrid Pulsed Laser Deposition — •Niklas Kohlrautz, Pia Henning, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

High- and medium-entropy materials (HEMs and MEMs) are known for their great multifunctional properties, such as ordered magnetism and promising catalytic behavior [1]. Moreover, tellurides are recognized for their novel magnetic properties, including room-temperature

ferromagnetism and large magnetic anisotropy, as well as catalytic potential [2][3]. Designing novel high-entropy tellurides opens new possibilities for discovering multifunctional materials. Toward the goal of synthesis of novel HEMs, we fabricated MEM tellurides (FeCrNiTe) via hybrid pulsed laser deposition (PLD). In this presentation, we will address the challenges in growing $(FeCrNi)_x Te$ and the detailed structural and physical characterization. FeCrNiTe films were synthesized on $SrTiO_3(001)$ substrates providing FeCrNi via the standard PLD process and Te through a molecular beam source, allowing easy Te stoichiometry control. Systematic studies of growth parameters yielded high-quality epitaxial thin films with elemental surface homogeneity. We are investigating the magnetic, electric and electrocatalytic properties of the films, comparing the results with the crystal structure.

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DS 13.26 Thu 18:00 P1

Thin Film Effects in Ultra-thin, MBE-grown In_2Te_3-Films — •Lucas Bothe[1], Maximilian Buchta[1], Felix Hoff[2], Timo Veslin[2], Christoph Ringkamp[2], Ka Lai Mak[1], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

InSbTe (IST) as an unconventional Phase Change Material is of significant interest in recent years. However, the related binary compound In_2Te_3 is less studied. With its small direct band gap and high absorption coefficient, it is an interesting candidate for e.g. photodetectors.

Here, a thin film series of In_2Te_3 was fabricated employing Molecular Beam Epitaxy (MBE) to achieve highly textured thin films. These films are characterized via XRD, RHEED and Raman spectroscopy. Next to the structural bulk values measured for the thickest In_2Te_3 sample, a decrease in the out-of-plane lattice constant by up to 0.4 A with decreasing film thickness is reported. The in-plane lattice constants however increase for thinner films. This trend with reduced film thickness contrasts known thin-film effects in metavalently bonded materials like Sb_2Te_3 or Bi, as In_2Te_3 is not expected to exhibit metavalency. Furthermore, the structural changes in the thin films are unlikely to arise from strain, given the Te-terminated Si surface promotes van der Waals growth, preventing alignment of the Si and In_2Te_3 in-plane lattice constants.

In addition, thickness-dependent vibrational properties were determined by Raman spectroscopy.

DS 13.27 Thu 18:00 P1

The interface wz-GaN/rs-ScN studied by depth profiling photoelectron spectroscopy — Fabian Ullmann[1,2] and •Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

Theoretical predictions show extreme high polarization gradients and polarization-induced surface charge densities at interfaces of rock salt ScN and wurtzite GaN.

Experimental investigation were made by depth profiling X-ray photoelectron spectroscopy (XPS) along the interface of rs-ScN and wz-GaN grown by molecular beam epitaxy (MBE).

DS 13.28 Thu 18:00 P1

Deposition of Cr self-intercalated $Cr_{1+\delta}Te_2$ thin films by Hybrid Pulsed Laser Deposition — •Pia Henning, Laura Pflügl, Anna Tschesche, Tobias Meyer, and Jasnamol Palakkal — Institute of Material Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

$Cr_{1+\delta}Te_2$ thin films exhibited an increased interest over the last few years, due to their tunable magnetic anisotropy and ferromagnetism with T_C ranging from 150 K to 350 K [1]. This tunability of magnetic properties is sensitively linked to the stoichiometry, governed by the self-intercalation of Cr species between $CrTe_2$ layers [1]. Therefore, the sensitive control of δ in addition with the insurance of high crystalline quality, with epitaxial and low defect growth, is crucial for a profound discussion and comparison of thin film properties. In this work, we used a hybrid pulsed laser deposition (PLD) unit attached with Te molecular beam source for growing high quality $Cr_{1+\delta}Te_2$ thin films [1]. We studied the influences of different growth parameter settings on the thin film quality and properties. We were able to carefully modify the δ and thickness of the films and investigated their correlation with the magnetic and electronic properties. This material system is a promising candidate for spintronics application due to room temperature ferromagnetism, anisotropic magnetoresistance and huge perpendicular magnetic anisotropy. Our findings manifest the advantages of this technique for depositing further novel transition metal chalcogenides. [1] A. Tschesche, P. Henning, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

DS 13.29 Thu 18:00 P1

Investigating Lateral Molecular Heterogeneity with Phase-Resolved Vibrational SFG Microscopy — •ben john, alexander p. fellows, tuhin khan, martin wolf, and martin thämer — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Understanding molecular heterogeneity at interfaces is crucial for applications in fields such as biophysics and materials science. Systems like lipid rafts in biological membranes or functionalized surfaces in microfluidics require techniques capable of resolving molecular structures, orientations, and compositions with high sensitivity and spatial resolution. Phase-resolved vibrational sum-frequency generation (vSFG) microscopy has emerged as a powerful tool to meet these needs, offering vibrational specificity, orientational sensitivity via second-order selection rules, and sub-micron spatial resolution through frequency upconversion. Despite its potential, traditional vSFG microscopy has faced significant technical challenges in detecting weak signals from monolayers and spatially mapping them. We address these limitations with an advanced phase-resolved vSFG microscope, which achieves improved signal-to-noise ratios and spatial resolution. Using this system, we successfully image phase-separated monolayers of mixed chiral lipids, revealing spatial heterogeneity in molecular orientations and packing structures. This breakthrough positions phase-resolved vSFG microscopy as a transformative approach for characterizing interfacial molecular systems, enabling deeper insights into the complex behaviors of molecular assemblies in both natural and engineered environments.

DS 13.30 Thu 18:00 P1

Structural and optical properties of β-Ga_2O_3 thin films obtained by spray pyrolysis — •Polina Shamrovska[1,2], Oleksandr Selyshchev[1], Narmina Balayeva[1], Volodymyr Kudin[2], and Dietrich Zahn[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

β-Ga_2O_3 thin films have gained significant research interest due to their wide bandgap, high thermal stability and breakdown voltage, making them suitable *e.g.* for UV photodetectors. Here, β-Ga_2O_3 thin films were deposited on c-plane sapphire substrates via spray pyrolysis, a cost-effective technique suitable for large-scale production. For deposition, we used $Ga(NO_3)_3$ dissolved in a 1 : 1 water-ethanol mixture or water with 1% polyethyleneimine, followed by annealing at 800 °C or 1000 °C. The films were characterized by SEM, AFM, Raman, XRD, spectroscopic ellipsometry, UV-vis spectroscopy, and electrical resistance measurements by the four-point probe.

The stoichiometric β-phase Ga_2O_3 films revealed a preferred $(\bar{2}01)$ orientation in agreement with previous results [1]. The samples showed transparency of up to 99% in the visible range and a sharp absorption edge in the UV range with bandgaps of 4.9 to 5.3 eV. The resistivity of the films was in the GΩ range. The results obtained reveal that spray pyrolysis allows the fabrication of highly crystalline, transparent, and high-resistive β-Ga_2O_3 films suitable for further studies as UV photodetectors.

[1] Akazawa, Housei, Vacuum, 2016, 123: 8-16.

DS 13.31 Thu 18:00 P1

"Green" Aqueous Synthesis and Characterization of Cu_2NiSnS_4 and Cu_2ZnSnS_4 Nanocrystal Thin Films — •Oleksandra Ivakhno-Tsehelnyk[1], Oleksandr Selyshchev[1], Serhiy Kondratenko[2], Volodymyr Dzhagan[3], Lukas Hertling[1], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes, Chemnitz University of Technology, 09107 Chemnitz, Germany. — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine. — [3]Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 03038 Kyiv, Ukraine.

We investigated thin films of Cu_2NiSnS_4 (CNTS) and Cu_2ZnSnS_4 (CZTS) nanocrystals (NCs) obtained by "green" colloidal synthesis [1,2]. This synthesis approach provides a way to non-toxic and scalable production for sustainable and low-cost light-absorbing nanomaterials. To assess the potential of thin films of these NCs for photovoltaic and

other possible applications, electrical studies are necessary. Colloidal NCs were deposited on glass substrates by spin coating and annealed at temperatures starting from 180 °C to obtain conductive thin films. Analytical techniques such as Raman spectroscopy, AFM, XRD, spectroscopic ellipsometry, and 4-point probe measurements were used to characterize their structural, optical, and electrical properties. We discuss the optical and electrical differences related to Zn-to-Ni substitution in the NC structure and establish the correlation between electrical properties of the films and elemental composition in both colloidal NCs and annealed films.

DS 13.32 Thu 18:00 P1

An in-situ μGISAXS growth study of CoFeB thin film on ion beam sculptured Si template — •Vishnu Narayan Manoj Kumar[1], Praveen Kumar Dubey[2], Prasanta Karmakar[3], Kristian A Reck[4], Benedikt Sochor[1], Yusuf Bulut[1], Thomas Strunskus[4,5], Franz Faupel[4,5], Stephan V Roth[1,6], Peter Müller Buschbaum[7], Ajay Gupta[2], and Sarathlal Koyiloth Vayalil[1,2] — [1]DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]UPES, Bidholi, Dehradun, India-248007 — [3]VECC, 1/AF, Bidhannagar, Kolkata -700064, India — [4]Chair for Multicomponent Materials, Department of Materials Science, Kiel University Kaiserstr. 2, 24143 Kiel, Germany — [5]Kiel Nano, Surface, and Interface Science, KiNSIS, Kiel University, Christian-Albrechts Platz 4, 24118 Kiel, Germany — [6]Division of Coating Technology, KTH Royal Institute of Technology, Teknikringen 48, 100 44 Stockholm, Sweden — [7]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, Garching 85748, Germany

In this work, the growth and structural evolution of CoFeB thin films deposited on nanopatterned Si templates prepared by N_2^+ ion beam irradiation has been done using in-situ micro GISAXS. Different growth regimes have been identified using appropriate growth models. Thin film is found to replicate the sawtooth ripple geometry of the templates up to a large extent of film thickness near 15nm. Strong uniaxial magnetic anisotropy has been observed in this system. Direction of magnetic easy axis is found to be changing with annealing.

DS 13.33 Thu 18:00 P1

Structure evolution of multi-component Ti-Nb-Zr-based thin films with Ag addition during heat treatment — •Anna Benediktová, Lucie Nedvědová, Zdeněk Jansa, Palaniappan Subramanian, Michal Procházka, and Ján Minár — University of West Bohemia, Pilsen, Czech Republic

Multicomponent and high-entropy alloys represent an intensively studied group of materials. Due to their potential to be chemically and structurally very stable, wear resistant and hard, they have also become the subject of study as biomaterials. Conventional metallic biomaterials usually have many disadvantages, including inadequate antibacterial properties leading to infections and possible implant loss. To improve the surface properties, thin films with different amounts of silver as an antibacterial agent were prepared by magnetron sputtering. Their structure in the as-deposited state and the evolution of the structure during heat treatment were analyzed in detail by diffraction techniques (XRD, SAED) and by scanning and transmission electron microscopy (SEM, TEM). The chemical states of the surface were investigated by X-ray photoelectron spectroscopy (XPS). The chemical stability of the films in phosphate buffered solution (pH ~ 7.4) was evaluated by electrochemical methods such as potentiodynamic polarization and electrochemical impedance spectroscopy.

DS 13.34 Thu 18:00 P1

Microscale Domain Structures in AlScN Thin Films — •Ella Dieball[1], Nicolas Hayen[1], Otto Lippmann[1,3], Philipp Jordt[1], Niklas Wolff[2], Lorenz Kienle[2], Fabian Westermeier[4], Michael Sprung[4], and Bridget Murphy[1,4,5] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Institute of Material Sciences, Kiel University, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [5]Ruprecht Haensel Laboratory, Hamburg, Germany

Thin films of Aluminium-Scandium Nitride (AlScN) are used as central components in magnetoelectric surface-acoustic wave sensors utilized extensively within the Collaborative Research Center 1261 "Biomagnetic Sensing".
High resolution XRD experiments were conducted at microfocus beamline P10 at PETRA III. Bragg diffraction on AlScN thin films grown on GaN was investigated at the [0 0 0 2], [0 0 0 4] and [0 1 -1 5] reflections. The material exhibits an unexpected domain structure on the μm scale, which is associated with Scandium-rich and Scandium-depleted regions.
Additional synchrotron experiments are in planning to further investigate AlScN, e.g. grazing incidence diffraction or absorption measurements around the Scandium K-edge.

DS 13.35 Thu 18:00 P1

In Operando Grazing Incidence Diffraction in AlScN Surface Acoustic Wave Sensors — •Otto Carlos Lippmann[1,2], Nicolas Hayen[1], Philipp Jordt[1], Jana Meyer[5], Fabian Lofink[5], Henrik Wolframm[4], Didier Wermeille[7], Laurence Bouchenoire[7], Florian Bertram[3], and Bridget Murphy[1,3,6] — [1]Institute of Experimental and Applied Physics, Kiel, Germany — [2]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [3]Deutches Elektronen Synchrotron, DESY, Hamburg, Germany — [4]Faculty of Engineering, Kiel, Germay — [5]Fraunhofer Institute for Silicon Technology ISIT, Itzehoe, Germany — [6]Ruprecht-Haensel Laboratory, Hamburg, Germany — [7]European Synchrotron Radiation Facility, Grenoble, France

Magnetic field sensors based on thin-film surface acoustic wave (SAW) technology are widely utilized in Collaborative Research Center 1261 "Biomagnetic Sensing". The use of Aluminium-Scandium-Nitride (AlScN) as the piezoelectric material allows for significant improvements in device sensitivity.
To investigate the microstructure of AlScN during the excitation of acoustic modes, an *in operando* setup was developed for high-resolution X-ray diffraction (XRD). This setup induces standing waves and allows the observation of diffraction patterns. A comparison of grazing-incidence diffraction (GID) of the [0 1 3] Bragg reflection between the stationary and operating state shows a shift in the signal peak position. Additional experiments are planned, along with the development of a new setup for time-resolved experiments. These efforts aim to enhance the understanding of SAW propagation in these materials.

DS 13.36 Thu 18:00 P1

Deterministic single ion-implantation of Er into thin film lithium niobate — •Maranatha Andalis, Reiner Schneider, and Klaus D. Jöns — Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP) and Department of Physics, Paderborn University, 33098 Paderborn, Germany

Incorporating rare earth ions (REIs) into lithium niobate-on insulators (LNOI) is of great interest in scalable photonic integrated circuits (PIC), enhancing the potential of LNOI with added functionalities enabled by the REIs. Erbium ions can be incorporated into LNOI using ion implantation and implemented at telecom wavelengths. Together with Ionoptika Ltd., we have customized a single ion implantation system called Q-One with up to 40 kV acceleration voltage. For most quantum applications, the site-selective implantation of a single REI is required. Our results show single Er ion implantation into LNOI with 85% efficiency using secondary electron emission detection. The Q-One single ion implanter, with its high-resolution mass-filtered focused ion beam, nanometer-precision stage, and choice of ion source, holds significant potential in deterministic ion implantation, crucial for scalable quantum technologies with REIs.

DS 13.37 Thu 18:00 P1

Impact of ITO electrodes on the electrical and optical properties of a smart window — •Rebecca Cizek[1], Florian Sutter[1], Stephan Heise[1], Kai Gehrke[2], Eckhard Lüpfert[1], and Robert Pitz-Paal[1] — [1]German Aerospace Center, Institute of Solar Research, Oldenburg, Almería, Köln, Germany — [2]German Aerospace Center, Institute of Networked Energy Systems, Oldenburg, Germany

This study investigates the impact of indium tin oxide (ITO) electrodes on the performance of smart windows utilizing reversible metal electrodeposition (RME). RME is a promising technique for fabricating electrochromic devices, offering dynamic control over light transmission. ITO electrodes, known for their high conductivity and transparency, play a critical role in facilitating the electrochemical processes that govern the reversible metal deposition and dissolution on the window surface. The effects of ITO electrode characteristics, such as conductivity, surface morphology, and transparency, are explored in relation to the electric and optical performance of the smart window. Long-term measurements are conducted with voltage applied over several hours to assess the durability and performance of the electrodes under operation.

DS 13.38 Thu 18:00 P1

Antibacterial activity of ZnO and Al doped ZnO nanocoatings — •Maria Stefanova[1], Dimitrina Petrova[1,2], Vladimira Videva[1], Dimitre Dimitrov[1,3], Nadia Todorova[4], and Vera Marinova[1] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]South-West University Neofit Rilski, Blagoevgrad, Bulgaria — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research Demokritos, Athens, Greece

Here we report on thin coatings of metal oxides (ZnO and ZnO doped with Al (AZO)) deposited by ALD technology. Their structural, surface-morphological and optical properties were investigated by AFM analysis, UV-Vis and fluorescence spectroscopy, as well as surface contact angle measurements. The antibacterial activity against Escherichia coli bacteria was evaluated in the dark and under ultraviolet light illumination. AZO nanocoatings were found to demonstrate more effective antibacterial action, mostly due to the improved sensitivity at UV spectral range as well as hydrophilicity in comparison with ZnO. The studied nanocoatings can serve as effective antimicrobial agents in a variety of applications.

Acknowledgements: This work is supported by the Bulgarian National Science Fund under the grant number KP-06-N-58/12 and the Research equipment of distributed research infrastructure INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science.

DS 13.39 Thu 18:00 P1

Chiral Induced Spin Selectivity Cooling — •Ohad Golan[1], Yossi Paltiel[1], and Ron Naaman[2] — [1]Hebrew University of Jerusalem, Jerusalem, Israel — [2]Weizmann Institute of Science, Rehovot, Israel

Chiral Induced Spin Selectivity (CISS) is a quantum phenomenon in which electron spins become selectively polarized as they pass through chiral materials. This effect enhances spin-dependent interactions without the need for external magnetic fields, playing a crucial role in various spintronic and chemical processes. Building on this principle, the Chiral Induced Spin Selectivity Cooling (CISSCO) effect exploits CISS to generate a temperature gradient across chiral materials. When current flows through a chiral system from a source to a drain, spin alignment at the source increases local entropy, leading to heating, while spin randomization at the drain reduces entropy, resulting in cooling. Unlike conventional thermoelectric and magnetocaloric effects, CISSCO requires no magnetic materials, enabling efficient and highly localized cooling. This groundbreaking mechanism has the potential to transform nanoscale heat management, offering an innovative solution for cooling micro- and submicron electronic devices.

DS 13.40 Thu 18:00 P1

NaCl-assisted TAC synthesis of MoSe2 films for optical humidity sensor applications — •Blagovest Napoleonov[1], Katerina Lazarova[1], Dimitrina Petrova[1,2], Vladimira Videva[1,3], Dimitre Dimitrov[1,4], and Vera Marinova[1] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]South-West University Neofit Rilski, Blagoevgrad, Bulgaria — [3]Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria — [4]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

We present the synthesis of MoSe2 through the Thermal Assisted Conversion (TAC) method with Mo liquid precursor solution composed of MoO3 dissolved in a 1:1 mixture of H2O and H2O2, with NaCl as an additive. The precursor solution enables controlled delivery of Mo during the TAC growth. The presence of NaCl influences the growth kinetics and crystallization during the annealing step. Raman spectroscopy, TEM, AFM and XPS measurements were employed for comprehensive material characterization, revealing the effectiveness of this precursor combination in synthesizing high-quality MoSe2 films. Based on optical reflectance measurements, the MoSe2 films demonstrate sensitivity to relative humidity changes by reflectance variation. These results led to the development of an optical humidity sensor, showcasing the material's potential in sensor applications. Acknowledgements: This work is supported by the Bulgarian Science Fund under the grant number KP-06-COST/15 under the COST Action CA20116 OPERA European Network for Innovative and Advanced Epitaxy.

DS 13.41 Thu 18:00 P1

Functionalization of Al-doped ZnO nanolayers for display applications — •Stefani Bogoeva[1], Vladimira Videva[1], Dimitrina Petrova[1,2], Vera Marinova[1], and Dimitre Dimitrov[1,3] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]Faculty of Engineering, South-West University, 2700 Blagoevgrad, BG — [3]Institute of Solid State Physics, BAS, 1784 Sofia, BG

The integration of highly transparent and conductive thin films into functional structures and devices plays an important role in the advancement of next-generation technologies. Here we report about Aluminum doped ZnO (AZO) thin films synthesized on different substrates using the atomic layer deposition (ALD) technique, which allows excellent conformality. The effect of post-deposition treatments on the optical and electrical properties of the films was studied using variety of characterization techniques.

Based on the above characteristics, integration of AZO layers in liquid crystal (LC) devices and Polymer Dispersed Liquid crystals (PDLC) structures are demonstrated, with measured electro-optical characteristics and response time. Implementation of AZO layers opens prospective applications for future ITO-free optoelectronics.

Acknowledgments The research was supported by the Scientific Research Fund project No. KP-06-*-58/12, as well as the distributed scientific infrastructure INFRAMAT, part of the National Roadmap of Bulgaria for scientific infrastructure, financially supported by the Ministry of Education and Science.

DS 13.42 Thu 18:00 P1

A high-field, high power instrument for (nonlinear) Terahertz Emission Spectroscopy — •Jonas Woeste[1,2], Nikola Stojanovic[2], Sergey Pavlov[2], Sergey Kovalev[3], and Michael Gensch[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany — [2]DLR - Institute of Optical Sensor Systems, Berlin, Germany — [3]Fakultät Physik, Technische Universität Dortmund, Dortmund, Germany

The quest to understand nonlinear terahertz phenomena has driven the development of advanced instruments towards the capability to detect faint terahertz transients with sub-cycle time resolution. The instrument presented here is optimized for a mJ-level laser amplifier operating at kHz repetition rates. It generates high-field THz pulses with peak fields of a few 100 kV/cm spanning frequencies from 0.3-1 THz. Using ultrashort NIR pulses for tilted-pulse-front pumping of a lithium-niobate crystal, pulse energies of up to 5 μJ are achieved. Demonstration experiments include studies on various doped semiconductors, graphene, and chip-integrated Dirac materials giving insights into different nonlinear and non-perturbative quantum phenomena.

DS 13.43 Thu 18:00 P1

Techno-Enviro-Economic Evaluation for Thin-film Solar Cells Integrated with Hybrid Renewable Energy System — •Tawfik Hussein — Mechanical Engineering Dep., National Research Centre (NRC), El Buhouth st.,Dokki, Cairo, Egypt

Thin-film solar cells (TFSC) have surfaced as a potentially viable substitute in recent years. TFSC have emerged as a transformative technology in the renewable energy sector, offering unique advantages such as lightweight construction, flexibility, and cost-effectiveness compared to conventional crystalline silicon photovoltaics.

The main objective of this study is to design an optimal hybrid renewable energy system (HRES) integrating TFSC in order to achieve efficient use of the available renewable energy sources (RES). Therefore, a HRES consisting of different RES integrated with TFSC is proposed to cover reliable electricity to a scientific farm in Egypt with technical, environmental, and economic evaluation. The research highlights the performance of TFSC under varying environmental conditions, emphasizing their superior efficiency in low-light and high-temperature scenarios. All the parameters, such as system performance, net present cost, and carbon emissions, are considered.

The results showed that the proposed TFSC delivers highly efficient energy generation at significantly lower costs compared to traditional configurations. From an environmental perspective, it achieves a significant reduction in carbon emissions and demonstrates improved sustainability.

DS 13.44 Thu 18:00 P1

Molecular packing and alignment of prototypical acenes in organic 2D-material heterostructures — •Jan Vincent Schreiber and Gregor Witte — Philipps-Universität Marburg, Molekulare Festkörperphysik, 35032 Marburg, Germany

Heterostructures comprised of thin films of organic molecules and two-dimensional materials, notably monolayers of transition metal dichalcogenides, are emerging as a promising class of systems for applications in organic electronics. Unlike metallic surfaces, two-dimensional materials interact with adsorbates primarily through van der Waals forces, resulting in substrate-adsorbate interactions comparable in strength to intermolecular forces. This delicate balance means that even minor variations in surface characteristics or growth conditions can significantly affect the relative molecular alignment. A systematic investigation of the molecular model systems pentacene and 5,7,12,14-pentacenetetrone allows comparison of the influence of electrostatic forces on the film alignment. Techniques ranging from scanning tunnelling microscopy to optical polarisation microscopy highlight the necessity of understanding these interactions across multiple length scales. We demonstrate that for most substrates, specific molecular orientations optimize the system's structural energy, a phenomenon known as van der Waals epitaxy. Our findings emphasize the need for rigorous structural studies to unravel the interplay between molecular structure and substrate properties.

DS 13.45 Thu 18:00 P1

Spectroscopy of organic dye/TMDC heterostructures — •Christoph von der Oelsnitz[1,2], Julian Schröer[1,2], Tim Völzer[1,2], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institut für Physik, Universität Rostock, Albert-Einstein-Straße 23, 18059 Rostock, Deutschland — [2]Department LL&M, Albert-Einstein-Straße 25, 18059 Rostock, Deutschland

Heterostructures composed of organic molecules adsorbed onto transition metal dichalcogenide (TMDC) monolayers can exhibit charge separation after optical excitation, making these systems promising candidates for optoelectronic applications. In this study, we investigate heterostructures consisting of the organic dyes copper phthalocyanine (CuPc) and 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) deposited onto TMDC monolayers and hexagonal boron nitride (hBN), with the latter serving as a non-interacting reference system. First, the preparation of the dye layers via thermal vapor deposition was calibrated and performed. Subsequently, we investigated the dye/TMDC and dye/hBN heterostructures using various spectroscopic methods. In the event of charge separation in the dye/TMDC system, photoluminescence quenching of the dye is expected.

DS 13.46 Thu 18:00 P1

Substrate-driven Molecular Orientation of BQQDI-based Organic Thin Films — •Jeya Vishva Jeyaraj Pandian and Gregor Witte — Philipps-Universität Marburg, FB Physik

Thin films of PhC_2-BQQDI, a high-performance n-type organic semiconductor, exhibit preferential molecular orientations depending on the substrate. On weakly-interacting amorphous SiO_2 substrates, the molecules adopt an upright orientation. Furthermore, a co-existence of thin-film phase was observed depending on the growth parameters, which is characterised by the increased molecular tilt angle with respect to the surface of the substrate. Notably, a domination of thin-film phase was observed at elevated temperatures. This phenomenon contradicts a commonly observed growth behaviour in organic thin films, whereby bulk phase prevails under such growth conditions. However, post-deposition annealing results in a transition from thin-film phase into bulk phase with significant dewetting. In contrast to SiO_2, on surfaces of alkali halides such as KCl, the molecules exhibit a recumbent orientation. Furthermore, an epitaxial growth was observed, driven by the templating effect of the underlying substrate. These findings pave the way for a phase-selective preparation of thin films of PhC_2-BQQDI which can be used to deepen the understanding of electronic transport in devices based on PhC_2-BQQDI.

DS 13.47 Thu 18:00 P1

The influence of stoichiometry on molybdenum oxide-based memristors — •Katerina Maskanaki[1], Gion Kalemai[2,3], Evangelos K. Evangelou[1], and Anastasia Soultati[2] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Institute of Nanoscience and Nanotechnology (INN), National Center for Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece — [3]Department of Physics, University of Patras, 26504 Patra, Rio, Greece

Transition metal oxides (TMOs) are a promising class of materials for neuromorphic computing and processing systems demonstrating a variety of resistive switching (RS) mechanisms. However, little is known about the correlation between its stoichiometry and RS. This study is focused on the development and characterization of molybdenum oxide memristors with different stoichiometry. Both, fully-stoichiometric (MoO_3) and sub-stoichiometric (MoO_{3-x}) molybdenum oxide devices showed good resistive switching behavior. However, the stoichiometric memristor exhibited better RS properties with endurance of 250 cycles, ON/OFF ratio $> 10^2$ and high retention of 2×10^4 s, compared to the poor RS behavior of the device based on the MoO_{3-x} film. This impressive memristive behavior could be attributed to the excess of oxygen vacancies in the case of fully-stoichiometric memristor in respect to the sub-stoichiometric MoO_{3-x} which play crucial role in the conductive behavior of the device. The high reproducibility observed in MoO_3-based memristor highlights their potential for practical applications and scalability.

DS 13.48 Thu 18:00 P1

In and ex situ detection of oxygen vacancies in HfO2 - advanced by PLD growth control and (HAX)PES spectroscopy — •Berk Yildirim[1], Seema Seema[1], Oliver Rehm[1], Pia Düring[1], Andreas Fuhrberg[1], Andrei Gloskovskii[2], Christoph Schlueter[2], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]DESY, Hamburg, Germany

Hafnium dioxide (HfO2) has emerged as a promising ferroelectric material, particularly suitable for non-volatile memory devices. Ferroelectricity in HfO2 is closely linked to oxygen vacancies (OV), but their direct experimental observation is challenging. This study uses tailored growth conditions to systematically control the OV concentration in HfO2 thin films as an essential prerequisite for their in and ex situ detection. In our pulsed laser deposition (PLD) system, parameters such as temperature, laser fluence, and oxygen partial pressure were varied to prepare HfO2 thin films with defined OV concentrations. In situ X-ray photoelectron spectroscopy (XPS) and ex situ hard X-ray photoelectron spectroscopy (HAXPES) provided detailed insight into OV distribution with different depths sensitivity, while structural properties were examined by in situ RHEED and ex situ X-ray diffraction (XRD) as well as atomic force microscopy (AFM). In and ex situ (HAX)PES analysis indicates a direct relationship between oxygen supply and the OV content via analysis of the Hf3+/Hf4+ spectral weight. In addition, the structural analysis points towards a systematic dependence between the onset of epitaxy and oxygen supply.

DS 13.49 Thu 18:00 P1

Oxygen vacancy mediated epitaxial superstructure thin film in tungsten sub-oxides — •Kyeong Jun Lee[1], Hyowon Seo[2], Yeong Gwang Kim[2], Yong-Jun Kwon[3], Bongju Kim[1], Minu Kim[1], Chan Ho Yang[3], Hyun Hwi Lee[4], Sang-youn Park[4], Gyungtae Kim[5], Jung-ho Kim[6], Young Jun Chang[2], and Seo Hyoung Chang[1] — [1]Department of Physics, Chung-Ang University, Seoul 06974, South Korea — [2]Department of Physics, University of Seoul, Seoul 02504, South Korea — [3]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, South Korea — [4]Pohang Accelerator Laboratory, POSTECH, Pohang 37673, South Korea — [5]National NanoFab Center, Daejeon 34141, South Korea — [6]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA

In metal oxides, oxygen vacancies are key to enhancing energy conversion and unconventional properties. Crystallographic shear (CS) planes in these structures are vital for electrochemical electrodes. While powders and polycrystals are well studied, research on single crystals or epitaxial films is essential to link oxygen vacancies with electronic and crystal structures. We fabricated epitaxial {103} CS superstructures in tungsten sub-oxides (Magnéli phases) on NdGaO3 (110)o substrates. X-ray scattering, AFM, and TEM confirmed epitaxial growth. W L3 RIXS revealed W6+ 5d0 and W6+ 5d1 states, showing oxygen vacancies' role in mediating superstructures and electronic properties.

DS 13.50 Thu 18:00 P1

Electronic structure of the TiO2/AlInP heterointerface studied by photoemission spectroscopy — •Mohammad Amin Zare Pour[1,2], Sahar Shekarabi[1], Jonathan Diederich[3], Negin Mogharehabed[2], Christian Höhn[3], Wolfram Jaegermann[4], Dennis Friedrich[3], Roel van de Krol[3], Agnieszka Paszuk[2], and Thomas Hannappel[1] — [1]Grundlagen von Energiematerialien, Technische Universität Ilmenau — [2]Paszuk group, Technische Universität Ilmenau — [3]Institut für solare Brennstoffe, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [4]Fachgebiet Oberflächen-

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Many world-record photoelectrochemical cells use AlInP as a window layer for selective electron transport passivated with TiO2, which is stable in electrolytes. The electronic and atomic properties of the TiO2/AlInP heterointerface in dependence to AlInP surface terminations to were examined. TiO2 was deposited by atomic layer deposition on various AlInP surface reconstructions and the TiO2/AlInP interface band diagram was experimentally examined. XPS/UPS studies reveal that TiO2 deposition reduces AlInP band bending, while remaining surface states pin the fermi level and still induce band bending towards the interface. Based on AlInP surface reconstruction, the valence band offset ranges from 1.7 to 1.9 eV. The presence of an oxide layer hinders the growth of TiO2 relative to clean surfaces. AlInP window layers are prevalent in III-V heterostructures, therefore mapping the TiO2/AlInP interface's electrical properties can optimize photoelectrochemical interfaces and more.

DS 13.51 Thu 18:00 P1

Resonance Raman and DFT analysis of structural and point defects in transparent conductive oxide SnO2:X (X=Ta, F) — •Lukas Prager[1], Carlos Romero Muñiz[2], Frans Munnik[1], Justus Haag[1], Ramon Escobar Galindo[3], and Matthias Krause[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Departamento de Física de la Materia Condensada, Universidad de Sevilla, Avda. Reina Mercedes s/n, 41012-Sevilla, Spain — [3]Departamento de Física Aplicada I, Escuela Politécnica Superior, Universidad de Sevilla, Virgen de África 7, 41011-Sevilla, Spain

Structural and point defects have a crucial influence on the electronic and optical properties of transparent conductive oxides. In this contribution we characterize different types of defects in SnO2:X (X = Ta, F) by the combination of laser-wavelength dependent Raman spectroscopy and state-of-the-art density functional theory (DFT) calculations using hybrid functionals.

Sn-vacancy- and O-interstitial-type point defects are found in transparent conductive SnO2:Ta thin films grown at 575 °C. These defects are responsible for strong, fingerprint-like Raman lines out of the phonon range of SnO2 [1], which are resonance-enhanced in the visible spectral range. The defects induce strong distortions of the electronic structure in the upper range of the valence band of Ta-doped SnO2. Moreover, the DFT calculation reveal a localized, molecular nature of the O interstitial and a delocalized nature of the Sn vacancy defect.

[1] M. Krause, et al., J. Mat. Chem. A 11, 17686-17698, (2023).

DS 13.52 Thu 18:00 P1

Ion Beam Sputter Deposition of Aluminium oxide Thin Films for electronic applications — •Prakrthi Alankaru Narayana[1,2], Aurelio García-Valenzuela[1], Jens Zscharschuch[1], Charlotte Kielar[1], Holger Lange[1], Claudia Neisser[1], Thomas Seyller[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Germany

Aluminium oxide (Al2O3) has drawn considerable interest from the research community due to its versatility in microelectronics particularly as a high-k dielectric in Complementary Metal Oxide Semiconductor (CMOS) devices. Ion Beam Sputter Deposition (IBSD), a physical vapor deposition method, facilitates the formation of Al2O3 thin films with fewer defects, improved composition, and better adhesion than compared to other physical deposition methods.

This work focuses on optimizing ion beam parameters to improve film properties such as stoichiometry, surface roughness, crystallinity, optical transmittance, and dielectric constant. Furthermore, the influences of oxygen flux and annealing on film properties have been investigated. To demonstrate the applicability of the deposited Al2O3 films, they have been utilized as a high-k dielectric material in metal-insulator-metal capacitors.

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[2] D. Niu et al. Surface and Coatings Technology 291, 318 (2016).

DS 13.53 Thu 18:00 P1

Band gap engineering of $SrNbO_3$ using anions — •Abhishek Sharma, Jasnamol Palakkal, and Christian Jooss — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Green energy is the demand of this generation for a better, eco-friendly future. Solar energy, being a renewable source can fulfill our demand through solar energy harvesting, which converts available sunlight to electrical energy. Transparent conducting oxide $SrNbO_3$ is a promising material for use in silicon tandem solar cells due to its wide bandgap (1.99 eV) and flexibility of the transparency window to be varied across different wavelengths using defects concentration [1]. Cationic and anionic defect engineering also varies this material's electrical conductivity from a metallic conductor to a ferroelectric insulator [2]. Upon introducing Sr vacancies, we changed the plasma frequency of $SrNbO_3$ from the visible light region (1.99 eV) to the near-infrared region (1.37 eV) [1]. In our ongoing work, we further vary the electrical and optical properties using anion modification in the form of oxygen defects and nitrogen anion introduction. A hybrid pulsed laser deposition unit with plasma sources for gases is being used carefully to control the anions in this materials system.

1. *Palakkal et al., arXiv:2410.01253.

2.*Chen. et.al., ACS Nano, 2017, 11, 12519-12525.

DS 13.54 Thu 18:00 P1

Thickness dependence of transport in thin crystalline FeTe films — •Paul Zhuromskyy, Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Iron chalcogenides present an intriguing material class for solid state physics; they have been shown to display antiferromagnetism, tunable superconductivity, inverted phase change behaviour, and unique interface effects when brought into contact with topological insulators. The layered compound FeTe has been predicted to be a topological semimetal. Although it has been the subject of numerous investigations, so far little attention has been given to the effects of nanoscale confinement below a thickness of 100 nm. Besides electrical transport, we have also analyzed optical and vibrational properties with regards to topological effects and phase transitions of FeTe for decreasing film thicknesses, from 80nm down to a few monolayers, and identified inflection points at which the phase transitions and conduction behaviour change due to confinement effects. Due to the importance of interfaces for topologically nontrivial materials, this presents a step towards the understanding of electronic phenomena in iron chalcogenides, as well as finding practical applications for FeTe in nanoelectronics. Our findings reveal that the complexity of solid-state systems makes them challenging to model but offers tunable parameters like quantum confinement to create novel phenomena and materials. Characterizing these dependencies helps uncover new connections and property design opportunities.

DS 13.55 Thu 18:00 P1

Charge Density Waves and resulting properties of polycrystalline CuTe Films — Johannes Holters, •Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Charge density waves (CDWs) are periodic modulations of charge density in materials, often coupled with structural distortions and electronic property changes. The layered transition metal monochalcogenide CuTe exhibits a CDW phase below 335 K in single crystals, accompanied by a Peierls distortion along its Te-chains, which confines electron transport to a quasi-1D channel. While this phenomenon has been extensively studied in bulk single crystals, its manifestation in polycrystalline thin films is less well characterized. Here, we investigate the CDW phase and topological properties of sputter-deposited CuTe thin films with varying thickness. We observe that the CDW transition persists in these films, and its characteristics are influenced by thickness and microstructure. By modeling the resistivity curves, we extract key physical parameters, like the CDW transition temperature and its broadening due to the grain size distribution. Further, we explore the topological semimetal (TSM) characteristics in the non-CDW state (T>335K), examining features such as magnetoresistance and the planar Hall effect. Our results highlight the robustness of the CDW in polycrystalline CuTe and its sensitivity to film structure, extending the understanding of CDW behavior beyond bulk crystals. These findings reveal the interplay between CDWs, TSMs and microstructure, offering potential for novel device applications.

DS 13.56 Thu 18:00 P1

Mechanical stress of Ge films upon ion irradiation — •Karla Paz Corrales[1], Aaron Reupert[2], Berit Marx-Glowna[3], Martin Hafermann[1], Elke Wendler[1], and Carsten Ronning[1] —

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Mechanical stress in thin films significantly affects the performance, reliability, and durability of optoelectronic components. Polycrystalline films are considered to be in a "stressed state" due the mismatch of the thermal expansion coefficients between the film and substrate. Amorphous Ge films (˜600nm) were deposited on fused silica substrates by magnetron sputtering. Subsequent annealing was performed at 600°C for 1h and 7h in vacuum to achieve crystallization. GIXRD patterns show peaks related to the polycrystalline Ge with preferred orientation along the [111] direction. Laser curvature measurements showed compressive stress for amorphous Ge-films, while the polycrystalline Ge samples became tensile stressed after annealing. In situ curvature measurements during ion-irradiation, using Au ions with 1.8 MeV on the polycrystalline Ge, show a decrease in stress with increasing irradiation fluence. Furthermore, optical measurements were performed after irradiation, and a reduction in the reflectance region of 450 to 650 nm and a shift of the absorption region up to ˜1000 nm were observed due to ion beam-induced defect formation.

DS 13.57 Thu 18:00 P1

Single-Phase Crystallization and Optimization for Optical and Electrical Properties of Sputtered In_3SbTe_2-SnTe Thin Films — •Zhengchao Zhu, Thomas Schmidt, Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide phase-change materials (PCMs) are known for their distinct differences in dielectric property i.e. $\epsilon(\omega)$ and electrical conductivity between their amorphous and crystalline states. This ability to rapidly switch between phases under light or electrical pulses makes them promising for applications in data storage and solar energy systems. One of the next-generation PCMs, In_3SbTe_2 (IST), exhibits a transition from dielectric to metallic behaviour when crystallized, a characteristic that spans the entire infrared spectrum and offers gigantic potential for advancing nanophotonic technologies. However, IST faces a limitation at high temperatures, where it decomposes into InSb and InTe, leading to reduced phase contrast and diminished performance. SnTe, with its similar lattice structure to IST, shows excellent miscibility with IST and can prevent phase separation. Never the leer, mixtures containing 30%-60% IST still exhibit tendencies of phase separation. This study aims to synthesize single-phase alloys using magnetron sputtering, evaluating phase separation across different stoichiometries. Subsequent investigations will focus on determining crystallization temperatures, electrical conductivity, and optical constants of the samples.

DS 13.58 Thu 18:00 P1

Bond Confinement Induced Tayloring of Optical Properties — •Thomas Schmidt, Peter Kerres, Felix Hoff, Julian Mertens, Yiming Zhou, Maria Häser, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide materials, such as GeTe and Sb_2Te_3, exhibit a broad range of properties that enable applications in thermoelectrics and phase change material (PCM) memory storage, where rapid and reversible switching between amorphous and crystalline states alters optical and electrical characteristics. Recent studies on textured chalcogenide thin films have focused on understanding structure-property relationships, particularly how properties evolve with film thickness. It is also explored how confinement influences atomic arrangement and bonding. Changes in bonding, particularly the transition from metavalent to covalent-like bonding, are linked to significant variations in material properties with decreasing thickness. In this work, we investigate the optical contrast of chalcogenide films by analyzing the thickness-dependent changes in the dielectric function. These findings are compared with the dielectric function of a mono-elemental system molecular beam epitaxy (MBE)-grown Bi films with thicknesses ranging from 2 to 30 nm to establish a link between bonding and optical properties.

DS 13.59 Thu 18:00 P1

Coherent Control of Optical Phonon Modes in Bi Thin Films Using Polarization and Double-Pulse Excitation — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], Felix Nöhl[1], Abdur Rehman Jalil[3], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

A new approach in the coherent control of optical phonon modes has been explored, enabling advances in material manipulation. By integrating polarization control with temporal modulation of double-pulse excitation, we show the selective and independent modulation of A1g and Eg phonon modes in a 12.5 nm bismuth thin film using a femtosecond pump-probe setup. This method takes advantage of the unique polarization dependencies of each phonon mode and quantum interference effects resulting from varying time delays between two pump pulses. The proposed approach is widely applicable to various materials and offers an unique level of active control over optical phonon excitation. This advancement could be relevant for emerging phononic technologies, such as nanoscale heat management, phononic data processing, and telecommunications. These applications are particularly vital for addressing the "THz gap" in the 1-10 THz spectral range, marking a crucial progress for the next generation of high-speed information transfer.

DS 13.60 Thu 18:00 P1

Ultra-fast exciton and charge carrier dynamics in monolayer MoS_2 seen in the transient spatial dielectric function — •Jakob Seyfarth[1], Andy Engel[2], Noah Stiehm[1], Younes Slimi[1], Lucas Krätschmer[1], Markus Olbrich[2], Theo Pflug[2], Alexander Horn[2], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Fachgebiet Technische Physik I, Technische Universität Ilmenau, Weimarer Straße 32, 98693 Ilmenau, Germany — [2]Laserinstitut Hochschule Mittweida, Schillerstraße 10, 09648 Mittweida, Germany

We present the charge carrier dynamics of monolayer MoS_2 on c-cut sapphire measured using pump-probe imaging reflectometry and interferometry with a spatial resolution of 0.65 micrometers and temporal resolution of 40 femtoseconds [1]. The time-resolved spatial dielectric function shows a diffusion which can be related to the dynamics of charge carriers. The dynamics can be attributed to specific events in the band structure of MoS_2 by comparing the results of a specific probe photon energy with previous time-resolved spectroscopic ellipsometry results [2]. References: [1] O. Herrfurth, T. Pflug, M. Olbrich, M. Grundmann, A. Horn, and R. Schmidt-Grund; Femtosecond-time-resolved imaging of the dielectric function of ZnO in the visible to near-IR spectral range; Appl. Phys. Lett. 115, 212103 (2019) [2] L. Krätschmer, Y. Slimi, L. Trefflich, S. Espinoza, M. Rebarz, J. Seyfarth, T. Pflug, M. Olbrich, N. Stiehm, B. Hähnlein, C. Sturm, A. Horn, J. Andreasson, M. Grundmann, S. Krischok, and R. Schmidt-Grund; Ultrafast Exciton and Charge Carrier Dynamics in Monolayer MoS2 Measured with Timeresolved Spectroscopic Ellipsometry; tbp

DS 13.61 Thu 18:00 P1

Anomalous Nernst effect in Fe-Ge-N thin films for power generation applications — •Robin Kidangan Paul[1], Imants Dirba[1], Oliver Gutfleisch[1], Jakub Vít[2], Petr Levinský[2], Kyo-Hoon Ahn[2], Karel Knížek[2], Markéta Jarošová[2], Jaroslav Kohout[2], Stanislav Mráz[3], Marcus Hans[3], and Jochen Schneider4[3] — [1]Functional Materials, Technical University of Darmstadt, Germany — [2]Institute of Physics of the CAS, Praha, Czech Republic — [3]Materials Chemistry, RWTH Aachen University, Aachen, Germany

With the growing demand for sustainable energy solutions, thermoelectric devices that convert heat directly into electricity have gained significant interest. While conventional thermoelectric devices based on the Seebeck effect are well-established, their complex designs and geometric limitations have hindered large-scale adoption. Anomalous Nernst Effect (ANE)-based devices have recently emerged as a promising alternative, offering simpler geometries and device flexibility. However, their adoption is constrained by lower efficiencies and output voltages compared to Seebeck-based counterparts. This study focuses on addressing these challenges by exploring materials with high ANE coefficients. Among the candidates, Fe4N has attracted attention due to its cost-effectiveness, nontoxicity, and tunability through elemental doping. DFT calculations of the Berry curvature indicate that doping Fe4N with Ge can enhance its ANE coefficient. In this work, thin films of doped Fe4-xGexN were fabricated onto MgO substrates using magnetron sputtering. Crystal structure, microstructure and transport properties are systematically characterized.

DS 13.62 Thu 18:00 P1

Resolving crystalline domains in an amorphous matrix via

APT — •Elias Hildebrand[1], Jan Köttgen[1], Ramon Pfeiffer[1], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Controlling crystallization from the amorphous state is critical for the development of new energy-efficient, non-volatile data storage technologies. The direct observation of crystalline nuclei is a challenging task because they are undetectable using classical X-ray diffraction.

In recent years, atom probe tomography (APT) has been established as an analytical technique for studying the microscopic structure of materials. Furthermore, it has been shown that for some chalcogenide materials (i.e., metavalently bonding materials), the difference between their amorphous and crystalline phases can be observed directly in APT data by utilizing the Probability of Multiple Events (PME).

In this project, APT is used to characterize amorphous and crystalline domains on a microscopic scale. The samples are produced using an in-house switching setup (the Phase Change Optical Tester) to reliably create crystalline regions within an amorphous matrix.

With this combination of techniques, we aim to achieve a better understanding of the crystallization mechanisms in chalcogenide glasses. This novel approach may help bridge the gap left by XRD measurements for small nuclei and thus improve control over crystallization and understanding of nucleation and growth on a nanometer scale.

DS 13.63 Thu 18:00 P1

Electrical switching dynamics of Ge-Sb-Te alloys for phase-change memories — •Alexander Kiehn[1], Ramon Pfeiffer[2], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Phase-change materials composed of Ge-rich Ge-Sb-Te alloys are promising candidates for next-generation phase-change memory (PCM) due to their nonvolatile nature, temperature stability, and fast switching speeds. These properties make them ideal for in-memory computing or applications in sensor systems, where fast, energy-efficient and reliable memory is crucial. However, in order to integrate PCMs into the usual semiconductor devices, it is necessary to reduce the switching voltage and current. This is influenced by the stoichiometry of the sputtered Ge-Sb-Te layer, which was varied in this study. Using industry-standard CMOS fabrication processes, chips were manufactured based on a confined cell PCM design. Based on the electrical switching results, trends in thermal stability and the resulting voltage requirements are clearly shown for increasing Ge content. These trends are supported by further investigating the crystallization behavior in optically-switched thin films.

DS 13.64 Thu 18:00 P1

Tailoring Metavalent Materials: Exploring the Structural and Functional Properties of $(GeTe)_x(SnTe)_{1-x}$ Alloys — •Jari Klinkmann[1], Lucas Bothe[1], Felix Hoff[2], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Metavalent materials have attracted significant interest due to their unique property portfolio, including medium electrical conductivities, high optical dielectric constants, large Born effective charges, and high Grüneisen parameters. GeTe and SnTe in particular are highly relevant for applications in thermoelectrics and phase-change memories. Here, we provide a comprehensive study of $(GeTe)_x(SnTe)_{1-x}$ alloys fabricated using molecular beam epitaxy (MBE). Structural characterization using x-ray diffraction alongside polarization-resolved Raman spectroscopy reveal the stoichiometry dependence of the rhombohedral-to-cubic phase transition, characterized by the loss of Raman-active modes in the cubic phase. Furthermore, coherent phonon investigations captured via femtosecond pump-probe spectroscopy detail the phase transition temperature evolution. Electrical and optical characterizations demonstrate the impact of stoichiometry on material properties, highlighting opportunities for tailoring these alloys for advanced technological applications.