DS 20: Poster

Time: Thursday 18:30–20:30 Location: P2

DS 20.1 Thu 18:30 P2

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 recently emerged as a transformative technology in renewable energy, offering advantages such as lightweight design, flexibility, and cost-effectiveness compared to conventional crystalline silicon photovoltaics. This study focuses on designing an optimal hybrid renewable energy system (HRES) that integrates TFSC to maximize the efficient use of renewable energy sources (RES). A proposed HRES, combining multiple RES with TFSC, was developed to supply reliable electricity to a scientific farm in Egypt, with full technical, environmental, and economic evaluation.

The research examines TFSC performance under diverse environmental conditions, highlighting their higher efficiency in low-light and high-temperature scenarios. System indicators including performance, net present cost, CO* emissions, and renewable fraction were analyzed. Results demonstrate that TFSC-based HRES delivers reliable, low-cost energy with notable environmental benefits. Compared to conventional systems, the proposed design achieves substantial reductions in both costs and carbon emissions, enhancing sustainability. These findings confirm TFSC as a promising solution for future renewable energy systems, addressing the increasing demand for affordable and eco-friendly power generation.

DS 20.2 Thu 18:30 P2

Structural and electronic characterization of sputtered MoSe2 and WSe2 thin films on ITO substrates using synchrotron-based XAFS/XRF techniques — •Sabit Horoz[1,2], Emre Timuçin Tabaru[1], Latif Ullah Khan[3], Messaoud Harfouche[3], and Ali Karatutlu[1,4] — [1]Sivas University of Science and Technology, Sivas, Türkiye — [2]Sivas Cumhuriyet University Nanophotonics Application and Research Center-CÜNAM, 58140 Sivas, Turkey — [3]SESAME, Allan, Jordan — [4]Bilkent University Ankara, Türkiye

Two-dimensional transition metal dichalcogenides (TMDs) such as molybdenum diselenide (MoSe2) and tungsten diselenide (WSe2) exhibit remarkable optoelectronic and catalytic properties. In this work, thin films of MoSe2 and WSe2 were fabricated on indium-tin oxide (ITO) substrates using a sputtering technique and analyzed at the SESAME Synchrotron facility through X-ray Absorption Fine Structure (XAFS) and X-ray Fluorescence (XRF) spectroscopy. XAFS results at the W L3- and Mo K-edges confirmed well-ordered W-Se and Mo-Se bonds, demonstrating crystalline TMD structures. Upon annealing up to 170 °C in air, partial oxidation led to the formation of WO3 and MoO3 phases, accompanied by a visible color change from silver to transparent. Complementary Raman, UV-VIS-NIR, and ellipsometric analyses supported these findings.

DS 20.3 Thu 18:30 P2

Investigation of a hygrosensitive polymer coating for colorimetric humidity sensing — •Ketrin Pavlova[1], Katerina Lazarova[1], Darinka Christova[2], Martina Docheva[1], and Tsvetanka Babeva[1] — [1]Institute of Optical Materials and Technologies "Acad. J. Malinowski" Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]Institute of Polymers, Bulgarian Academy of Sciences, Sofia, Bulgaria

A thin coatings of newly synthesized branched copolymers of poly(vinyl alcohol) comprising graft poly(N,N-dimethylacrylamide) with different side chains were studied as sensitive media for environmental changes of the relative humidity (RH). Spin-coating method was applied to deposit the thin films of both copolymers on Si-substrates, followed by temperature heating. Reflectance spectra of the samples were measured and then used to determine coating's thickness and optical constants. Sensing abilities of the coatings when exposed to different humidity level in range 5-95 RH% were examined and parameters such as hysteresis H and thickness change Δd were calculated. Possible application of the coatings for colorimetric detection is demonstrated.

DS 20.4 Thu 18:30 P2

Sputtered germanium absorbers for building-integrated semi-transparent photovoltaics — •Nico Ruskaup[1], Kai Gehrke[1], Stephan Heise[2], and Martin Vehse[1] — [1]Institut für Vernetzte Energiesysteme, Deutsches Zentrum für Luft- und Raumfahrt e. V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg — [2]Institut für Solarforschung, Deutsches Zentrum für Luft- und Raumfahrt e. V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg

Architectural glass facades worldwide typically utilize solar-control coatings deposited in inline magnetron sputter coaters to prevent buildings from excess solar heating. To use the electricity-generating potential of these facades, we aim to enable the glass industry to integrate photovoltaic functionality into their glazing using existing production lines. This requires a semi-transparent, fully sputtered thin-film solar cell. As a first step, here we demonstrate sputtered ultra-thin germanium absorber layers for semi-transparent solar cells. We compare their optoelectronic properties and their microstructure with established reference layers deposited by plasma-enhanced chemical vapor deposition (PECVD) and identify sputter-process conditions that yield germanium absorbers with PECVD-comparable properties suitable for device integration. We present a sputtered germanium layer built into a solar cell, which delivers a power conversion efficiency of 2.8%. These results demonstrate that sputtered germanium is a viable absorber for thin-film photovoltaics and represent an important step towards an industrially sputtered semi-transparent solar cell for window applications.

DS 20.5 Thu 18:30 P2

Enhanced Ferroelectric Behavior in NH4Cl-Doped SnO2/Perovskite Multilayer Memristors — •Katerina Maskanaki[1], Evangelos Evangelou[1], and Anastasia Soultati[2,3] — [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 Electrical & Computer Engineering, Hellenic Mediterranean University (HMU), Heraklion 71410, Crete, Greece

Perovskite-based materials have emerged as promising candidates for neuromorphic computing due to their diverse conduction mechanisms and tunable electronic properties. This study is focused on the development and characterization of multi-layered memristors with the structure ITO/SnO2:NH4Cl/RbCsMAFAPbI3/P3HT/Al. A reference device employing a pristine SnO2 layer was also fabricated to compare the memristive behavior to the modified devices incorporating an NH4Cl-doped SnO2 nanocomposite layer in various concentrations. All configurations exhibited stable memristive switching; however, the NH4Cl-modified devices demonstrated significantly enhanced ferroelectric behavior, achieving endurance over 200 switching cycles and robust data retention exceeding 10^3 s. The high reproducibility and scalability of these perovskite memristors highlight their strong potential for next-generation neuromorphic and memory applications.

DS 20.6 Thu 18:30 P2

How Matrix-Mediated Osmotic Forces Govern Spatio-Temporal Dynamics and Spreading in Two-Species Biofilms — •Anthony Pietz[1], Uwe Thiele[1], and Karin John[2] — [1]University Münster, Münster, Germany — [2]University Grenoble Alps, Grenoble, France

Biofilms are thin films of bacterial communities encased in a self-produced polymeric matrix that thrive on immersed or moist surfaces [1]. The matrix confers the biofilm mechanical resistance and drives an osmotic influx of nutrients rich water into the biofilm.

While the osmotic spreading of biofilms with only one species has been extensively studied, much less is known about how matrix-mediated osmotic forces influence the spatio-temporal organization and spreading dynamics in multi-species communities. Experiments on two-species mixtures of matrix producers / non-producers show that the latter becomes confined to the advancing biofilm edge [2].

We numerically investigate the dynamics of such a two-species biofilm where the matrix-producing species attractively interacts with the matrix. Our description supplements a thermodynamically consistent thin-film approach for a passive suspension by bioactive growth terms. We analyse the resulting spatio-temporal dynamics and identify conditions under which multispecies and monospecies biofilms develop.

[1] Wilking et al. Biofilms as complex fluids. MRS Bulletin 36: 385, 2013. [2] Yan et al. Extracellular-matrix-mediated osmotic pressure drives Vibrio cholerae biofilm expansion and cheater exclusion. Nature Communications 8: 327, 2017.

DS 20.7 Thu 18:30 P2

Coherent control in size selected semiconductor quantum dot thin films — •Victor Kärcher[1,2], Tobias Reiker[1], Pedro F. G. M. da Costa[3], Andrea S. S. de Camargo[4,5], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, 48149 Münster, Germany. — [2]Insititute of Physics, University of Münster, 48149 Münster, Germany. — [3]São Carlos Institute of Physics, University of São Paulo, São Carlos, SP 13566-590, Brazil. — [4]Federal Institute for Materials Research and Testing (BAM), 12489 Berlin, Germany. — [5]Friedrich-Schiller University Jena (FSU), 07743 Jena, Germany.

We introduce a novel technique for coherent control that employs resonant internally generated fields in CdTe quantum dot (QD) thin films at the L-point. The bulk band gap of CdTe at the L-point amounts to 3.6 eV, with the transition marked by strong Coulomb coupling. Third harmonic generation ($\lambda = 343\,$nm, h$\nu = 3.61$ eV) for a fundamental wavelength of $\lambda = 1,030$ nm is used to control quantum interference of three-photon resonant paths between the valence and conduction bands. Different thicknesses of the CdTe QDs are used to manipulate the phase relationship between the external fundamental and the internally generated third harmonic, resulting in either suppression or strong enhancement of the resonant third harmonic, while the nonresonant components remain nearly constant. This development could pave the way for new quantum interference-based applications in ultrafast switching of nanophotonic devices.

DS 20.8 Thu 18:30 P2

Ion slicing of gallium phosphide — •Otto Arnold[1,2,3], Tobias Bucher[1], Katsuya Tanaka[1,2,3,4], Muyi Yang[1,2,3,4], Carsten Ronning[1], and Isabelle Staude[1,2,3,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — [3]Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany — [4]Max Planck School of Photonics, Germany

Gallium phosphide (GaP) has unique non-linear and quantum optical properties, such as second harmonic generation and spontaneous parametric down-conversion. For integrated optics, preparing the single crystalline GaP on a low reflective index material would be useful, as the reflective index scales with the mode confinement of the enhanced near-field. So far, GaP thin films are grown epitaxially or with MOCVD, which are both expensive and complicated. An alternative approach is ion slicing, where a helium-irradiated GaP is bound to a borosilicate glass. We fabricated high quality GaP thin-film in (100) and (110) crystal orientation on glass, with a thickness of 760 (40) nm. Energy-dispersive X-ray spectroscopy (EDX) and Rutherford backscattering spectrometry (RBS) characterization of the fabricated thin-films allow us to further optimize the irradiation profile and bonding parameters towards best optical performance for further nanofabrication of resonant meta-surfaces operating in the visible and near-infrared.

DS 20.9 Thu 18:30 P2

Piezoelectric coatings on Fiber Bragg Gratings for electric field measurement — •Florian Schmidbauer and Jens Ebbecke — Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach

Monitoring high-voltage systems is gaining increasing importance. Conventional sensors often rely on electrical components that exhibit cross-sensitivities and require electrical wiring, which can pose a source of interference in certain applications. In addition, the physical dimensions of sensor heads can limit their usability.

An alternative approach employs Fiber Bragg Gratings (FBGs) coated with piezoelectric materials. Through the piezoelectric effect, mechanical deformation of the piezoelectric layer induces strain in the FBG, resulting in a measurable shift of its resonance wavelength. This type of sensor offers several advantages, including electrical passivity, a compact form factor, and the capability for remote and rapid signal interrogation via optical fibers.

This work presents the current progress in the development of such a sensor. Barium Titanate ($BaTiO_3$) was selected as the piezoelectric material due to its high piezoelectric coefficient and more environmentally friendly profile compared to PZT. The coating was successfully applied using two different methods: sol-gel dip coating and pulsed laser deposition. Potential application areas and opportunities for further design optimization are also discussed.

DS 20.10 Thu 18:30 P2

Thermoelectric-based position-sensitive detector — Jun Peng, Lucas Rave, Pai Zhao, Rakshith Venugopal, Kristian Deneke, Stefanie Haugg, Robert H. Blick, and •Robert Zierold — Center for Hybrid Nanostructures, University of Hamburg, Germany

Precise positioning is a never-ending goal in both fundamental science and technology. Conventional position-sensitive detectors (PSDs), which rely on lateral photoelectric effects in semiconductor junctions, are inherently restricted in operating temperature and are often unsuitable for detection beyond the optical regime. Here, we present a new detector architecture, the thermoelectric-based position-sensitive detector (T-PSD), that extracts spatial information solely from heat conduction and thermoelectric conversion. Specifically, the device incorporates an ALD-deposited Al-doped ZnO (AZO) thermoelectric thin film on an isotropic substrate, where Seebeck voltages measured across multiple electrodes encode the position of an incident heat spot. It can detect single heat spots arising from various energy sources, including electromagnetic radiation, electrons, and macroscopic mechanical heat. The thin-film design enables sub-micrometer spatial resolution in 1D configurations, while a two-ratio voltage decoding scheme provides robust and intensity-independent localization in 2D devices. Furthermore, the T-PSD exhibits broad temperature compatibility and is particularly well suited for high-energy beams, which remain challenging to localize with existing PSD technologies.

DS 20.11 Thu 18:30 P2

Research Infrastructure Access in NAnoscience & nanotechnology (RIANA) — •Ryan Yang — Helmholtz-Zentrum Dresden-Rosendorf, Dresden, Germany

RIANA is a Horizon Europe-funded consortium of seven Analytical Research Infrastructures in Europe (ARIE) comprising of 69 research facilities that offer open, curiosity-driven research in nanoscience and nanotechnology. By integrating advanced capabilities within Europe in simulation, material synthesis, nanofabrication, characterization, and analysis, RIANA provides a single-point entry for users to perform targeted and impact-orientated investigations.

Users can simply submit a single application to access any of the nanoscience infrastructures within RIANA. A comprehensive service, anchored by 21 Junior Scientists and supported by a panel of senior facility experts will guide users through technique selection, experimental operation, data analysis and publication. Parallel Innovation Services tailor access for industry (especially SMEs) helping mature technologies, raise TRLs, and scale production processes. The Smart Science Cluster (SSC) network of on-site Junior Scientists ensures hands-on support at every research stage, from experiment design to result interpretation. Specifically, users requiring beam-time among other methods of research can take advantage of RIANA and the FIB aspects of their projects will be delegated to the RADIATE network such as the HZDR*s Ion Beam Center.

My poster will introduce this EU project and how potential users can tap into this resource.

DS 20.12 Thu 18:30 P2

Tailoring of MoO3 Thin Films by Irradiation with Energetic Heavy Ions — •Islam Al-Hamad[1], Ayman El-Said[1], Mohammad Al-Kuhaili[1], Shavkat Akhmadaliev[2], and Stefan Facsko[2] — [1]Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In recent years, energetic heavy ions have been used to modify the physical properties of various materials [1]. In this study, we investigate the influence of irradiation of molybdenum trioxide (MoO_3) thin films with MeV ions of various parameters [2]. The films were deposited on fused silica using thermal evaporation technique. After irradiation, the films were characterized using optical spectroscopy and XRD techniques, showing the effectiveness of ion-irradiation in tuning the films optical and structural properties by varying ion beam parameters. This is highly important for the design of advanced metal oxide materials for sensing, switching, and energy applications.

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Beam Center at the Helmholtz-Zentrum Dresden-Rossendorf e. V., a member of the Helmholtz Association. A.S. El-Said acknowledges the support by KFUPM, Saudi Arabia (Project: ISP24236).

[1] A.S. El-Said, S. Rao, S. Akhmadaliev, S. Facsko, Phys. Rev. Appl. 13, 044073 (2020). [2] R. Sivakumar, et al., J. Phys.: Condens. Matter 19, 186204 (2007).

DS 20.13 Thu 18:30 P2

Quantifying surface/H-plasma interactions via in-situ observation of metal - insulator transition (MIT) in rare earth perovskites ($MNiO_3$) — •Balázs Antalicz[1], Sophia Sahoo[2], Parikshit Phadke[1], Roland Bliem[1], and Gertjan Koster[2] — [1]ARCNL, Materials & Surface Science for EUVL, Science Park 106, 1098 XG Amsterdam, The Netherlands — [2]University of Twente, Inorganic Material Science Group Hallenweg 23, 7522 NH Enschede, The Netherlands

In 'green' plasma reactors and semiconductor manufacturing, reactive H species clean surfaces, but also induce degradation, e.g. via blistering or embrittlement. To retain device performance, low-cost & complexity exposure monitoring is required – which faces fundamental challenges.

To solve this, materials with strong response to hydrogenation are of interest. For example, Pt-dissociated H_2 was shown to induce MIT in $MNiO_3$ perovskites, which was accompanied by an up to 10^7-fold electrical resistance increase. Because H-plasma contains multiple preactivated species, we anticipate simpler sensor designs are possible, without the Pt catalyst.

Using an accelerated plasma exposure tool, we then demonstrate MIT in epitaxially grown, Pt-free $NdNiO_3$. X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) shows partial Ni^{3+} reduction, and loss/alteration of crystallinity. Further results explore re-settability by annealing in O_2, and correlate O 1s XPS spectra with crystal-field theory, structure changes, and the onset of the insulator state.

DS 20.14 Thu 18:30 P2

Distributed Bragg Reflector-Enhanced Grating Coupler on SiON-Doped Silicon Platform for 905 nm Using Particle Swarm Optimization — •Metehan Ari[1], Iremnur Duru[1], Ali Karatutlu[1,2], and Timuçin Emre Tabaru[1] — [1]Sivas University of Science and Technology — [2]] Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University

A vertical grating coupler operating at 905 nm was designed on a silicon oxynitride-doped silicon (SiON-Si) platform for on-chip LiDAR. For the first time, the SiON-Si layer served as the core of a grating structure. The material exhibited a refractive index of 2.27, CMOS compatibility, and negligible two-photon absorption, with its electronic structure confirmed via soft X-ray absorption spectroscopy at the HESEB beamline (SESAME).

To enhance performance, a Distributed Bragg Reflector (DBR) consisting of three alternating SiON-Si/SiO* layers was integrated beneath the grating to suppress substrate leakage. Design optimization using Particle Swarm Optimization (PSO) and FDTD analysis demonstrated that the DBR increased coupling efficiency from ~35% to 53%. Consequently, the optimized device achieved 53% (-2.76 dB) efficiency for TM-polarized vertical coupling at 905 nm. Fabricating both the grating and waveguide within the same SiON-Si layer eliminated heterogeneous interfaces, maintained single-mode behavior, and validated the platform's potential for integrated photonic circuits.

DS 20.15 Thu 18:30 P2

XRD Data Analysis and Curve Fitting Using Differential Evolution in Python — •Simon Lorch, Tobias Pollenske, and Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Precise evaluation of X-ray diffraction (XRD) data is essential for understanding thin-film and interface structures at the atomic scale. In this contribution, we present a Python-based framework for automated fitting and quantitative analysis of experimental diffraction data using Differential Evolution (DE) as a global optimization strategy. The method minimizes the difference between measured and simulated intensity curves by evolving parameter sets such as layer thickness, density, and interfacial roughness toward the global minimum of an error function. Unlike conventional structure-factor-based approaches, the model deliberately omits detailed atomic scattering factors and instead focuses on the optimization of macroscopic parameters to reproduce the experimental curve shape. This allows a robust and efficient fitting of complex multilayer systems even in cases where structural details or phase information are incomplete. Compared to traditional gradient-based approaches, DE shows superior robustness against local minima and enables reliable fitting of complex multilayer systems with correlated parameters. The implementation allows user-defined boundary conditions, parallel evaluation of population members, and integration of physical models for scattering amplitude and Debye-Waller damping. This open and modular approach shows how evolutionary algorithms can make XRD data analysis more reproducible and accurate.

DS 20.16 Thu 18:30 P2

Stress Evolution in Gold Thin Films Under Ion Irradiation — •Jasmin Kahl[1], Karla Paz[1], Berit Marx-Glowna[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Helmholtz-Institut Jena, Fraunhoferstr. 8, 07743 Jena, Germany

Gold thin films are important for applications requiring mechanical stability and radiation tolerance in optoelectronic devices. This work investigates the stress evolution of polycrystalline Au films irradiated with He, Si, Ag, and Au ions at various energies and fluences. Insitu stress measurements during irradiation show that the as-deposited films are pre-stressed and the mechanical stress increases under irradiation producing a tensile stress. SEM and FIB cross-section images confirm that this stress increase is associated with grain growth, which depends strongly on the ion species. Grain growth increases local density and generates tensile stress because the films are constrained by the substrate. Large grains are advantageous in applications such as electrical interconnects and microstructures, as they reduce electromigration and optical losses. X-ray diffraction reveals structural damage, lattice distortion, and possible crystallite reorientation, while AFM shows increased surface roughness due to sputtering. These results highlight the strong influence of ion species and irradiation conditions on Au thin films, guiding the optimization of gold-based components in demanding environments.

DS 20.17 Thu 18:30 P2

Structural and magnetic properties of epitaxial Fe-Sn thin films. — •Benedikt Eberts[1], Franz Weidenhiller[2], Matthias Küss[1], Lin Chen[2], Christian Back[2], and Manfred Albrecht[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Magnetic Weyl semimetals exhibit strong spin-orbit coupling and nontrivial band structures, enabling efficient field-free manipulation of magnetic states through spin-orbit torque [1], which makes them highly attractive for spintronic applications. Among them, the ferromagnetic Weyl semimetal Fe3Sn2 and the antiferromagnetic Dirac semimetal FeSn provide a good platform for investigating spin-orbit-driven phenomena. Both compounds crystallize in a layered Kagome lattice, where the corner-sharing triangles lead to strong frustration. In this work, we have grown high-quality epitaxial thin films of FeSn and Fe3Sn2. The films were deposited at elevated temperatures using magnetron sputtering. A seed layer system of Pt and Ru on Al2O3(0001) substrates was used to promote epitaxial growth. Thin films of varying thickness were prepared and characterized using XRD, AFM, MFM, SEM, TEM, and SQUID magnetometry. FMR measurements on Fe3Sn2 revealed low damping and the expected sixfold symmetry associated with the Kagome lattice. These thin films will next be used to study charge-spin conversion processes [2]. [1] Lyalin, I. et al., Nano Lett. 21, 6975-6982 (2021) [2] Zhang, S.-L. et al., Phys. Rev. Lett. 123, 187201 (2019)

DS 20.18 Thu 18:30 P2

Single-crystalline Ni thin films as templates for epitaxial growth of 2D materials — •Paula Vierck, Audrey Gilbert, Domenik Spallek, Jonas Lähnemann, and J. Marcelo J. Lopes — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

Hexagonal boron nitride (h-BN) offers multiple interesting applications as a component in heterostructures with other 2D materials, for example as a passivation layer or a tunnel barrier in electronics. However, the synthesis of large-scale high quality h-BN required for such applications remains challenging, and the vast majority of the van der Waals heterostructures having h-BN as a building block are still prepared using mechanically exfoliated h-BN flakes.

To serve as a substrate for large-scale h-BN grown by molecular beam epitaxy (MBE), in this work, we investigate the synthesis of Ni films on Al_2O_3(0001) and MgO(111) using magnetron sputtering. The structure and morphology of the Ni films is characterized using X-ray diffraction (XRD), atomic force microscopy (AFM) and electron backscatter diffraction (EBSD). The structural quality of the Ni films is improved by systematically varying experimental parameters such as substrate temperature, sputtering power, film thickness and the post-growth annealing temperature, finally resulting in single crystalline Ni films with (111) orientation only.

DS 20.19 Thu 18:30 P2

Structural and optical properties of undoped β-Ga2O3 thin films deposited by ultrasonic spray pyrolysis — •Polina Shamrovska, Narmina Balayeva, and Dietrich Zahn — Technische Universität Chemnitz, Chemnitz, Germany

β-Ga2O3 thin films have gained significant research interest due to their wide bandgap, high thermal stability and breakdown voltage, making them suitable for e.g. UV photodetectors. Here, β-Ga2O3 thin films were deposited on c-plane sapphire substrates via ultrasonic spray pyrolysis, a cost-effective technique suitable for large-scale production. The deposition was performed with Ga(NO3)3 dissolved in a 1 : 1 water-ethanol mixture at a substrate temperature of 190 °C and post-deposition annealing was performed at 1000 °C. The films were characterized by Raman, AFM, XRD, optical transmittance, and conductivity measurement.

The stoichiometric β-phase Ga2O3 films revealed a preferred (-201) orientation in agreement with previous results [1]. The samples show transparency of up to 85% in the visible range and the conductivity increases with increasing film thickness. The results obtained reveal that ultrasonic spray pyrolysis allows the fabrication of highly crystalline and transparent β-Ga2O3 films suitable for further studies as solar-blind UV photodetectors.

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

DS 20.20 Thu 18:30 P2

Analyzing interface properties of energy materials using thin film model systems materials — •Julius K. Dinter, Anja Henss, and Matthias T. Elm — Institute of Experimental Physics I, Justus-Liebig University, Heinrich-Buff-Ring 16, D-35392, Giessen, Germany

Energy materials used in modern electrochemical devices must provide sufficiently high ionic and electronic conductivity, as both ions and electrons are stored and/or transported during device operation. However, most ionic conductors exhibit negligible electronic conductivity, and the opposite is true for typical electronic conductors. Consequently, artificial mixed-conducting composite materials are often prepared by combining ionic and electronic conducting compounds. These artificial mixed ionic-electronic conductors exhibit a large number of internal interfaces, which strongly influence charge storage and transport in the composite.

To clarify the role of such interfaces on overall electrochemical behavior, thin-film model systems with controllable and well-defined interfaces are essential. In this work, we present the fabrication of artificial mixed-conducting thin films based on lithium-ion- and oxygen-ion-conducting oxides prepared by pulsed laser deposition. Structural and compositional characterization using XRD, Raman spectroscopy, time-of-flight secondary ion mass spectrometry, and electrochemical impedance spectroscopy confirms the successful deposition and integrity of the designed model systems.

DS 20.21 Thu 18:30 P2

InAsP quantum emitters on InP with single-photon emission from O- to C-band up to 80 K — •Yiteng Zhang[1], Doaa Abdelbarey[1], Markus Etzkorn[2], Zenghui Jiang[1], Ankita Choudhary[1], Tom Fandrich[1], Arijit Chakraborty[1], Chenxi Ma[1], Pengji Li[1], Xin Cao[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,3], and Fei Ding[1,3] — [1]Leibniz University Hannover, Institute of Solid State Physics, Appelstraße 2, 30167 Hannover, Germany — [2]Technische Universität Braunschweig, Laboratory for Emerging Nanometrology (LENA), Langer Kamp 6a, 38106 Braunschweig, Germany — [3]Leibniz University Hannover, Laboratory of Nano and Quantum Engineering, Schneiderberg 39, 30167 Hannover, Germany

We grow InAsP nanostructures on InP(001) by high-temperature annealing under arsenic flux followed by controlled cooling. In situ RHEED and ex situ AFM/TEM show that this sequence produces coherent, compositionally graded InAsP islands. Low-temperature micro-photoluminescence reveals spectrally isolated emission lines from individual emitters covering the telecom O- to C-bands; power dependence and second-order correlations under continuous-wave excitation show excitonic behaviour and clear antibunching with g2(0)<0.1, confirming single-photon emission. Temperature-dependent measurements indicate that single-photon emission persists up to temperatures above 80K.

DS 20.22 Thu 18:30 P2

Investigations of point defects in Nb3Sn thin films for SRF application — •Sebastian Klug[1], Maik Butterling[2], Eric Hirschmann[1], Andreas Wagner[1], and Maciej Oskar Liedke[1] — [1]Institute of Radiation Physics, HZDR, Germany — [2]Reactor Institute Delft, Delft University of Technology, The Netherlands

Bulk Niobium cavities are the state-of-the-art option to realizes high-performing linear particle accelerators. To achieve even better performance and lowering operational costs, a thin film approach with different superconducting materials is necessary. Nb3Sn coatings are promising candidates because of its high superconducting transition temperature (Tc up to 17 K). Magnetron sputtering is a very suited PVD method which provides high deposition rates and a large spectrum of deposition parameters optimization. Maximizing the transition temperature and the lower critical magnetic field Hc1 could be correlated to the structure and point defects in thin films like vacancies, their agglomerations and pores. To study this effect, positron annihilation spectroscopy (PAS) with a high sensitivity to small void-like defects is used. PAS provides non-destructive and depth-resolved information of defect type, size and density as well as their local atomic chemistry in many material types like metals, polymers, ceramics and semiconductors. In this contribution, investigations on magnetron sputtered Nb3Sn thin film samples will be presented. A special focus is set to positron annihilation spectroscopy to study the influence of different deposition parameters on defect formation and the resulting superconducting performance.

DS 20.23 Thu 18:30 P2

Surface Investigations of Ga-polar wz-GaN Grown by Plasma Assisted MBE — •Abdul Qadir Shabaz[1,2], Anees Ul Hassan[1,2], 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

Since very high polarization gradients are predicted for wz-GaN/rs-ScN interfaces, well-oriented, clean Ga-polar wz-GaN surfaces are required in order to grow rs-ScN on top of this layer in a ultra high vacuum to achieve high quality interfaces. These thin layers were grown via plasma-assisted molecular beam epitaxy on 6H-SiC substrate. X-ray photoelectron spectroscopy (XPS), ultra violet photo electron spectroscopy (UPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were performed to investigate electronic structure, composition and morphology of the surfaces.

DS 20.24 Thu 18:30 P2

Bonding and properties in NiTe-NiTe$_2$: Transition from normal metal to Dirac semimetal — •Christian Stenz[1], Kethusan Karunanathan[1], Paul Zhuromskyy[1], Kijoon Cheong[1], Tim Bartsch[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

We investigate the evolution of bonding and electronic properties across the NiTe-NiTe$_2$ system, focusing on the transition from conventional metallic behavior in NiTe to topological Dirac semimetallicity in NiTe$_2$. NiTe exhibits isotropic bonding between Ni d- and Te p-electrons, characteristic of a normal metal. In contrast, NiTe$_2$ forms a layered structure with a pseudo van-der-Waals gap and weak Te p-p interactions, hosting Dirac nodes near the Fermi level that give rise to non-trivial topological surface states and linear magnetoresistance. By tuning the Ni content in sputtered thin films, we control the interlayer coupling mediated by Ni d-electrons, enabling systematic exploration of the transition between these bonding regimes. Using density functional theory and tight-binding calculations, we analyze how additional d-electrons influence the band structure, Berry curvature, and Dirac cone formation in NiTe$_2$. Correlations between these electronic changes and material properties - such as optical and electrical conductivity, linear positive magnetoresistance, emergence of soft anharmonic bonds and bond rupture behavior - are examined.

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Development of sacrificial layers grown on rare-earth scandate substrates for epitaxial KNN/KTN layer transfer — •Diana Avetisyan, Jeremy Maltitz, Jutta Schwarzkopf, and Jens Martin — Leibniz-Institut für Kristallzüchtung

Future technologies in sensing, communication, and computing require integrated devices with ultra-low-loss processing, precise control of photons, electrons, and spins, fast switching, broad frequency operation, and strong nonlinearities. Silicon photonics alone cannot meet these demands, making hybrid integration via layer transfer a promising approach. A promising material is sodium-doped potassium niobate, potassium tantalate, and their alloys to enable integration with photonic and acoustic devices. These materials exhibit exceptional electro-optic coefficients, nonlinear Kerr coefficients, piezoelectric coupling coefficients, and elasto-optic coefficients. The project focuses on transferring freestanding sodium-doped potassium niobate membranes onto SiO_2/Si substrates. This involves growing sodium-doped potassium niobate on a sacrificial layer/substrate stack, chemically etching the sacrificial layer, and transferring the membrane. Different substrates and sacrificial layers are explored to achieve crack- and wrinkle-free membranes. The membranes are characterized for surface topography, crystalline structure, ferroelectric, piezoelectric, and electromechanical properties for future device applications.

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Formation and protection of two-dimensional electron gases at SrTiO3 interfaces via redox reactions — •Shi-Hui Liu, Georg Hoffmann, and Roman Engel-Herbert — Paul-Drude-Institut für Festkörperelektroni, Berlin, Germany

Strontium titanate (SrTiO3) has been the workhorse for development of new physical phenomena over decades. Recently, new momentum was generated when the formation of a two-dimensional electron gas (2DEG) via oxygen scavenging effect at the SrTiO3/AlOx interface was observed, i.e. oxidation of the deposited metal-layer upon reduction of the SrTiO3 [1]. However, depending on the Al layer thickness, these 2DEGs degrade over time due to diffusion of oxygen from the gas phase through the AlOx layer refilling the vacancies.

In this work, amorphous aluminum layers with thicknesses ranging from 0.5 to 2.5 nm were deposited on TiO2-terminated SrTiO3 (001) substrates using molecular beam epitaxy. The complementary methods of in-situ x-ray photoelectron spectroscopy, and capacitance-voltage measurements were performed to monitor the interfacial redox reaction and to identify the spatially confined conduction channel, respectively. Since the 2DEG remains stable only for a limited time within an optimum aluminum layer thickness, strategies for protecting and stabilizing the 2DEG will be pointed out.

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E-Beam Evaporation of thin metal and oxide films on Al_2O_3 (0001) — •Laurenz Hüffmeier, Tobias Pollenske, and Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin metal and oxide films are used in numerous fields of application, particularly in optics, electronics, and energy applications. With the increasing importance of these technologies, the requirements for these films are also rising in order to improve their properties. Precisely manufactured films with well defined structural and physical properties are required, as even minimal deviations in thickness or structure can significantly impair device performance. A suitable method for the growth of such layers is physical vapor deposition (PVD), which enables the controlled deposition of a wide variety of materials under high vacuum conditions. Here, electron beam evaporation (EBPVD) is advantageous since extremely clean films can be deposited and high evaporation rates of up to a few micrometers per second are possible. Hence, in this work, ultrathin magnesium oxide, praseodymium oxide, cobalt, and platinum films were deposited on insulating Al_2O_3 (0001) substrates using EBPVD. The structural properties of the resulting layers were analyzed by XRR. XPS measurements were performed on all films to examine their near-surface chemical composition. For the cobalt layers deposited with different emission currents, XPS was performed both in situ and ex situ to investigate the influence of atmosphere conditions on the oxidation states.

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Towards Low-Temperature ALD of Topological Insulator Sb_2Te_3 — •Luise Merkwitz[1,2], Paul Pöhler[1,2], Steffen Ziller[1], Knut Ulbrich[1], Marek Ulbrich[1], Sebastian Lehmann[1], and Kornelius Nielsch[1,2] — [1]Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Dresden, D-01069 Dresden, Germany

Low-Temperature ALD expands the range of applications for ALD enabling not only the deposition of thin films on temperature-sensitive substrates but also the possibility of a more ressoure-efficient setup and reaching advantages in material conformity and less sample defects.

We have designed, constructed and developed a state-of-the-art Low-Temperature ALD reactor for high-quality thin films. Our previous results demonstrate the technical functionality and reproducibility of known Low-Temperature ALD processes. In addition, our latest results reveal a never before published Sb_2Te_3 synthesis which we consider to be a highly promising Room-Temperature ALD process.

DS 20.29 Thu 18:30 P2

Using layered metamaterials in spin - ventil structures as a basis for artificial neural network — •Vladimir Boian[1], Cătălin Cimbir[1], and Vladimir M Fomin[2] — [1]Technical University of Moldova, Institute of Electronic Engineering and Nanotechnologies, Chisinau, Moldovau — [2]IET, Leibniz IFW Dresden, Dresden, Germany

Elaboration of a superconducting artificial neural network (ANN) the most promising solution in the design and development of non-von Neumann architectures. There are two main components of ANN: the nonlinear switch neuron constituting a spin valve, and the linear connection element the synapse. This study presents the results of computer modeling of superconducting spin valves on the base of Josephson Junction with weak link prepared from artificial magnetic metamaterials, and of superconducting synapses, based on hybrid layered structures superconductor/ferromagnet. The proximity effect in a superlattice formed by superconducting Nb nanolayers and ferromagnetic Co layers with different thicknesses and coercive fields is analyzed both theoretically and experimentally. In this sense, they can be applied as tunable kinetic inductors for the design of ANN synapses. Metamaterials based on Nb and Co nanolayers are a very promising class of artificial magnets for superconducting spintronics and quantum computing. The use of artificial neural networks with a radically reduced consumption of electricity are increasingly appreciated worldwide.

DS 20.30 Thu 18:30 P2

From Localised to Delocalised Charge Carriers: An Optical Investigation on Metal-Insulator Transitions — •Thomas Schmidt[1], Navjot Bamrah[2], Liron B. Michael[2], Ricardo P. M. S. Lobo[3], 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 — [3]LPEM, ESPCI Paris, CNRS, PSL University, 75231 Paris, France

Understanding metal-insulator transitions (MITs) has been a central topic in solid-state physics and materials science for decades. Various theoretical frameworks describe these transitions in terms of critical charge carrier densities (Mott MIT) or electron localisation induced by disorder (Anderson MIT). Typically, electrical conductivity measurements or their temperature-dependent derivative (TCR) are used to distinguish metallic from insulating behavior.

In this work, we propose an alternative approach based on optical spectroscopy. Reflectance spectra were recorded over a broad spectral range using a Fourier-transform infrared (FTIR) spectrometer. The optical functions were subsequently obtained through modeling of the measured data. Our analysis focuses on the evolution of the Drude response in the optical conductivity, which directly reflects the dynamics of free charge carriers. The Drude feature, defined by the ratio of the plasma edge to the scattering rate, provides valuable insight into the material-specific degree of electron (de)localisation and thus offers an alternative perspective on MITs and their relation to chemical bonding.

DS 20.31 Thu 18:30 P2

Investigating the Anisotropy of Optical Phonons in Ultrafast Optical Pump-Probe Experiments — •Felix Nöhl[1], Felix Hoff[1], Jonathan Frank[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

Phonons are quantized lattice vibrations closely linked to bond strength and atomic arrangement. A well-established tool to study incoherent optical phonons in frequency domain is Raman scattering. Ultrafast lattice dynamics and coherent phonons, capable of modulating macroscopic physical properties, are of interest to emerging research fields. In ultrafast optical pump-probe experiments, coherent optical phonons can be excited and directly measured in the time domain via transient changes in reflectivity. Due to their pronounced phononic response, bismuth and tin selenide were used to further explore the excitation and detection of coherent phonons. A pump polarization scheme for our optical pump-probe setup was implemented and polarization resolved pump-probe and Raman measurements compared. Clear symmetries were observed, highlighting the influence of the lattice structure. This improves our understanding of coherent phonon anisotropy in optical pump-probe measurements and enables modulation of the detected signal by changing the pump polarization.

DS 20.32 Thu 18:30 P2

Optimization of Reactive Ion Etching processes with Optical Emission Spectroscopy — •Daniel Breuer, Bich Nguyen, Teresa Wessels, and Markus Kaiser — Helmholtz Nano Facility, Forschungszentrum Jülich, Jülich, Germany

In modern technology, devices on the scale of micro- to nanometers play an important role. In the fabrication of those devices, the dry etching process is essential to structure them. Hereby the reactive ion etching technology has been established due to its very selective and anisotropic etching. To achieve reproducible results, process control is crucial. For this purpose, optical emission spectroscopy (OES) is employed to observe the spectra of the plasma during the process. Here, OES is used to ensure thorough cleaning of the RIE chamber after etching by defining the spectra of a clean chamber. Parameters, e.g. etching gas and time, are investigated with respect to their effect on chamber cleanliness. Finally, suggestions for a rigorous cleaning procedure are given. In addition, the endpoint detection is examined on a Si wafer with 200 nm SiN. Using OES, we aim to stop the plasma immediately when the SiN is etched through to prevent damage to the Si. We implement an endpoint detection by observing the characteristic line of the CN molecule, which is a typical product of the chemical etch reaction. The effects of various system parameters on the plasma, e.g. coupled power, chamber pressure and gas flow, are studied, as well as endpoint detection settings. In conclusion, a precise analysis of the plasma via OES allows us to specifically control the etching process.

DS 20.33 Thu 18:30 P2

Optimizing Erbium Luminescence in Silicon Nitride for Integrated Photonics via Oxygen Codoping and Thermal Annealing — •Felix Mania[1], Sören Lerner[1], Jiale Sun[2], Zheru Qiu[2], Xinru Ji[2], Tobias Kippenberg[2], and Carsten Ronning[1] — [1]Friedrich-Schiller Universität, Helmholtzweg 3, 07743 Jena, Germany — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Erbium-doped fiber amplifiers revolutionized long-haul optical communications, thereby establishing erbium ions as promising candidates for amplification in integrated circuits. However, their practical application in integrated photonics is currently limited by low luminescence efficiency. In this study, we utilize ion implantation into ultralow-loss silicon nitride (Si_3N_4) and investigate the influence of oxygen codoping and thermal annealing on the formation of Er-O complexes, thereby modifying the local crystal field of the erbium ions within the host matrix. Specifically, we examine the effects of varying oxygen doping concentration and annealing temperature via photoluminescence and lifetime measurements. These findings provide a critical optimization strategy for CMOS-compatible erbium-based emitters essential for future photonic integration.

DS 20.34 Thu 18:30 P2

Domain Transfer from Simulation to Experimental Neutron and X-ray Reflectivity Data Using Probabilistic Generative Models — •Jeyhun Rustamov[1], Ritz Aguilar[1], Vedhas Pandit[1], Nico Hoffmann[2], and Jeffrey Kelling[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Helm & Walter IT-Solutions, Dresden, Germany

Machine learning (ML) models trained on simulations often fail to generalize to experimental data in neutron and X-ray reflectivity analysis. Furthermore, determining thin film parameters from reflectivity curves is an inherently ambiguous inverse problem. To address this, we employ conditional normalizing flows (cNFs) with a β-Variational Autoencoder (β-VAE) embedding network to learn the full distribution of physical parameters instead of single estimates.

To further improve performance on experimental data, we systematically explore three strategies for bridging the simulation-experiment domain gap: fine-tuning with labeled experimental data, utilizing generative models to create realistic synthetic data, and a novel physics-informed method. The proposed method incorporates a differentiable forward function based on the kinematic approximation to guide the generation of sample parameters via physics-informed loss during bidirectional training of cNFs.

Our approach distinctly leverages unlabeled experimental reflection data to address cNF performance challenges on real-world reflectivity measurements. Additionally, this methodology can be broadly applied to other inverse problems with similar domain-transfer challenges.

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A Kramers-Kronig Consistent, Parameter Free, Probabilistic Dielectric Function Model — •Noah Stiehm[1,2], Stefan Krischok[1], Rüdiger Schmidt-Grund[1], and Jana de Wiljes[2] — [1]Technische Physik I, TU Ilmenau, Germany — [2]Mathematics of Data Science, TU Ilmenau, Germany

Utilizing a Bayesian probabilistic modeling approach to approximate the full posterior probability density $p(\theta \mid y)$ of a model's parameters θ given data y can provide greater insight into the model's performance and parameter uncertainties than point estimates provided by classic, deterministic optimization algorithms.

Here we present a parameter free dielectric function model, that might be used in a Bayesian modeling context as a substitute for the well known B-spline models. Our approach is based on Gaussian processes (GP), which are a flexible class of random functions, that enable numerical sampling in an efficient manner. We utilize a GP to model the time-domain response function $\chi(t-t')$ as a latent function, from which the dielectric function $\varepsilon(\omega)$ is constructed via a discrete Fourier transform. The resulting dielectric function is therefor Kramers-Kronig consistent by construction. We implement approximate and exact (depending on available compute resources) sampling strategies to include our model in different Bayesian modeling frameworks which utilize either Markov Chain Monte Carlo (MCMC) or particle filter methods. We demonstrate our model's performance in scenarios with significant uncertainties: a sample with a concentration gradient of a AgAl alloy, and pump-probe transient ellipsometry data.

DS 20.36 Thu 18:30 P2

Tunability of optoelectronic properties of the alpha-phase MoO3 thin films — •Zhihua Yong, Lars Steinkopf, Marin Rusu, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Alpha-phase MoO3 is widely used as a large bandgap hole transport layer (HTL) in solar cells due to its high work function, good hole conductivity and stability. For an appropriate energy level alignment with the active layer, the optoelectronic parameters of the MoO3 layers must be fine tuned. In this work, we fabricate uniform as well as combinatorially synthesised MoO3 films via Pulsed Laser Deposition on fused silica substrates in the temperature range of 350*480oC. The film thicknesses were targeted at approximately 15 nm, as usually applied for HTLs, and confirmed by X-Ray Reflectivity measurements. All films were found to be polycrystalline and contained only the α-phase with an orthorhombic crystal structure (Pbnm space group), as observed by X-Ray Diffraction and Raman Spectroscopy. Electronic properties of the MoO3 films were investigated by combining Kelvin probe (KP) measurements and photoelectron yield spectroscopy (PYS) under inert N2 atmosphere at ambient pressure. We show by means of KP-PYS studies that the ionisation energy and work function of the films can be fine tuned between 5.72 to 6.10 eV and 5.72 to 6.00 eV, respectively, by varying the deposition temperature. That results in a fine variation of the valence band maximum with respect to Fermi level. The degenerate state of the films is observed for deposition temperatures equal or higher than 425°C.

DS 20.37 Thu 18:30 P2

Heterodyne detection of the second harmonic signal in THz pump - optical probe experiments — •Sergei Ovcharenko, Alexey Melnikov, and Georg Woltersdorf — Institut für Physik, Martin-Luther-Universität Halle, 06120 Halle (Saale), Germany

Broadband Terahertz (THz) radiation is a widely used for resonant excitation of magnon modes or spin waves in magnetic materials. Furthermore, studying the THz emission from ferromagnetic (FM) materials allows us to investigate elementary processes in ultrafast spintronic. However, experimental investigation of such effects requires broadband THz detection: the commonly used sampling in electro-optical crystals is limited by phonon absorption, Zeeman-torque sampling requires accurate determination of the magneto-optical constants of a specific FM sample. An alternative approach is the detection of the THz field-induced second harmonic (TFISH) signal, based on third-order nonlinearity $\chi(3)$ in ambient air gases. Heterodyne detection, interference between the TFISH and SH light from a reference source, allows retrieval of the full THz pulse profile. The SH heterodyning technique is also applicable to extract weak SH signals, related to THz-induced magnetization dynamics in thin films. Our work reveals a phase modulation effect in the heterodyne TFISH signal: the air gap between TFISH and reference SH sources alters the detected THz pulse shape and spectrum through propagation effect in presence of the THz field. Using the developed instrument, we performed test experiments on heterodyne SH detection of THz-induced magnetization dynamics.

DS 20.38 Thu 18:30 P2

In_2Te_3 as a Covalent Spacer in GeSbTe-based Phase Change Superlattices — •Lucas Bothe[1], Maximilian Buchta[1], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), FZJ, Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Superlattices (SL) containing GeSbTe are promising material systems to overcome typical shortcomings of Phase Change Materials (PCM) by reducing the reset current by an order of magnitude. The reason for the increased energy-efficiency of SLs remains unclear. Typically, two metavalent materials, e.g. $GeSb_2Te_4$ and Sb_2Te_3, are used in superlattices to achieve superior switching performance. It is debated that Sb_2Te_3 plays a major role in achieving this performance increase. In this work however, Sb_2Te_3 is exchanged with In_2Te_3, replacing a metavalent with a covalent sesqui-chalcogenide to investigate its influence on the switching performance. In a first step, this work presents the growth of $GeSb_2Te_4/In_2Te_3$-SLs via MBE. XRD, RHEED, SEM and EDX were employed to characterize the samples. Pronounced Laue Fringes and clearly visible SL satellite peaks in the XRD-scans demonstrate the excellent sample quality and allow for exact characterization of the achieved SL-stacking. RHEED data allows the characterization of the coupling between $GeSb_2Te_4$ and In_2Te_3, which appears to be weak but not strictly of van-der-Waals character. As a next step the samples will be optically switched with a laser set up to compare the switching characteristics to those of $GeSb_2Te_4/Sb_2Te_3$-SLs.

DS 20.39 Thu 18:30 P2

Electrical switching dynamics of Ge-Sb-Te alloys for phase-change memories — •Alexander Kiehn[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

Off-stoichiometric 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 data storage, where fast, energy-efficient and reliable memory is crucial. However, in order to integrate PCM into standard semiconductor devices, it is necessary to reduce the switching voltage and current. This is greatly influenced by the composition of the sputtered Ge-Sb-Te layer, as well as the contact electrode material. Using CMOS-compatible fabrication processes, chips were manufactured based on a confined cell PCM design with new TaN contacts. Based on the electrical switching results, trends in thermal stability and the resulting voltage requirements are shown for different alloys. Further analysis also shows the SET and RESET speed as well as endurance of the devices.

DS 20.40 Thu 18:30 P2

Optimizing Crystallization Kinetics and Reducing Stochasticity of the Phase-Change Materials Sb2Se3 and Ge2SeTe through Controlled Crystalline Interface Growth — •Ramon Pfeiffer, Ramon Schmidmeier, Laura Gundermann, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide phase-change material (PCM) alloys such as Antimony Triselenide (Sb2Se3) and Germanium Selenide Telluride (Ge2SeTe) can be switched repeatedly with low optical losses, making them interesting contestants for integrated photonic circuits. However, by switching from the predominately investigated as-deposited phase these materials are characterized by a relatively slow crystallization speed and high stochasticity. To address these shortcomings, we investigate methods such as the recrystallization from differently melt-quenched phases and a crystalline ring. The later approach, allows for controlled growth from a crystalline interface. An increase of crystallisation speed and decrease of stochasticity is verified by a pump probe setup and through Electron Backscatter Diffraction (EBSD) measurements respectively.

DS 20.41 Thu 18:30 P2

Hard X-Ray Momentum Microscope Measurements of $SrCoO_x$ Thin Films at Beamline P22 — •Volkmar Koller, Sourav Chowdhury, Sergii Chernov, Andrei Gloskovskii, and Christoph Schlueter — Photon Science | DESY Hamburg

Emerging memory devices are a possibility to reduce electricity expenditure in the future compared to established complementary metal-oxide-semiconductors CMOS. For instance the Mottronic is based on a topotactic phase transition TPT associated with a metal-insulator transition MIT, instead of a manipulation of charges like in semiconductors. This might allow a further miniaturization of devices.

Here we show the Hard X-Ray Momentum Microscope HarMoMic at the beamline P22 of the PETRA III synchrotron at DESY as tool to monitor the electronic and crystalline structure of materials showing a TPT. Based on Hard X-ray Photoelectron Spectroscopy HAXPES the HarMoMic probes angle resolved the bulk electronic structure of single crystalline samples. Thus, the electronic band structure and X-ray photoelectron diffraction patterns XPD can be measured. From the XPD patterns the crystalline structure of a material can be determined by comparing it to simulations (Kikuchi Diffraction patterns).

As model system we show measurements of $SrCoO_x(001)$ thin films grown via PLD on Nb-doped $SrTiO_3(001)$. Upon the application of an electric bias it is electrochemically oxidized from $SrCoO_{2.5}$ (Brown-Millerite, insulator, antiferromagnetic) to $SrCoO_{3-\delta}$ (Perovskite-like, metallic, ferromagnetic) undergoing a TPT.

DS 20.42 Thu 18:30 P2

Intercalation of thin Fe-films at the Graphene/SiC Interface — •Niels Rösch[1,2], Fabian Göhler[1,2], Rico Ehrler[1,2], Susanne Wolff[1,2], Olav Hellwig[1,2], and Thomas Seyller[1,2] — [1]Technische Universität Chemnitz, Institut für Physik, 09126 Chemnitz — [2]Forschungszentrum für Materialien, Architekturen und Integration von Nanomembranen, 09126 Chemnitz

The intercalation of graphene on silicon carbide (SiC) with different materials is an extensively studied field of research. The intercalation of metals into the graphene/SiC interface offers a route to tune the structural, electronic and magnetic properties of the system [1,2].

In the present study, we demonstrate the successful intercalation of iron (Fe) between graphene and SiC. 4H-SiC(0001) substrates were used to prepare the buffer layer (BL) precursor by polymer assisted sublimation growth (PASG) [3]. Intercalation was carried out under ultra-high vacuum (UHV) conditions by depositing 2 nm Fe atop the BL precursor at 300 °C, followed by an annealing at 750 °C for 30 min.

The successful intercalation of iron at the BL/SiC interface was confirmed by photoelectron spectroscopy and electron diffraction. Magnetic characterization via superconducting quantum interference device magnetometer (SQUID) revealed that the intercalated Fe layer exhibits ferromagnetic behavior.

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[3] M. Kruskopf et al., 2D Mater. 3 (2016) 041002.

DS 20.43 Thu 18:30 P2

High-Fermi velocity massless carriers in a triangular monolayer of Sb — Bing Liu[1,2], •Kilian Strauss[1,2], Philipp Eck[2,3], Jonas Erhardt[1,2], Tim Wagner[1,2], Philipp Kessler[1,2], Cedric Schmitt[1,2], Lukas Gehrig[1,2], Stefan Enzner[2,3], Martin Kamp[1,2], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,3], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Two-dimensional (2D) quantum materials with high Fermi velocities are key candidates for ballistic transport and high-speed electronics. However, few 2D systems have the potential to demonstrate Fermi velocities exceeding that of graphene, remaining at the level of prediction. Here, we report the successful synthesis of a triangular monolayer of antimony (Sb) on the wide-gap semiconductor SiC. Using combined angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) in combination with density functional theory (DFT), we reveal orbital filtering that isolates broad-bandwidth, massless p_x and p_y states, yielding a compensated Fermi surface with an ultrahigh Fermi velocity surpassing that of pristine graphene. Linear dichroism in ARPES measurements confirm the orbital polarization of these high-velocity bands. This makes the triangular antimonene a compelling platform for next-generation quantum and high-speed electronic technologies.

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Interfacial electronic structure of molecular adsorbates on WS2 and doped MoSe2 — •Carolin Sabrina Schüle, Michael Lämmerhofer, Joschua Bueble, Louisa Adlung, and Heiko Peisert — Institut für Physikalische und Theoretische Chemie Universität Tübingen, Germany

MoSe2 and WS2 are layered transition metal dichalcogenides (TMDCs) and promising alternative to conventional semiconductor materials. We studied interface properties of different molecules on MoSe2 and WS2. In the case of MoSe2 also p- and n-doped substrates were studied. Comparably weakly interacting phthalocyanines (CoPc, MnPc, CoPcF16) were compared to strong electron acceptors (HATCN, C60). It is known that opotoelectronic properties of TMDCs such as MoS2 can be tuned by transition metal phthalocyanines (TMPCs), depending strongly on the central metal atom of the phthalocyanine,[1], the mechanism, however, is not completely understood. Generally, for TMDCs two different interaction channels are possible: Interaction via the central metal atom and the macrocycle. It is shown that the different ionisation potential of the molecules affect the size of interface dipoles, as well as a band bending in the bulk substrates. However, the role of interface states is not negligible. Also, the doping level of MoSe2 have an influence on the strength of the interaction, although no integer charge transfer might be expected. [1] DOI: 10.1021/jacs.1c07795

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Wannier-orbital Transient Polaron Localisation for electron and spin transport in organic semiconductors — •Nisarg Trivedi, Maximilian F.X. Dorfner, Michel Panhans, and Frank Ortmann — TUM School of Natural Sciences and Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München

Transport in organic semiconductors is governed by a complex interplay between comparable energy scales of electronic coupling, thermal disorder, and electron-vibration interactions, making it difficult to describe within a unified framework. Building on the hybrid Transient Polaron Localization (TPL) model proposed by Hutsch *et al.* (npj Comput. Mater. 8, 228, 2022), we introduce an efficient extension using Wannier orbitals as a localized and orthonormal basis, enabling accurate treatment of charge transport in extended pi -conjugated systems which also allows us to generalise the framework for spin transport.

DS 20.46 Thu 18:30 P2

A Dual Time-Scale KMC-MD Approach for Simulating Self-Assembly Kinetics of Polyalanine α-Helix Monolayers — •Bo-Yue Zeng[1], Hadis Ghodrati Saeini[1], Sibylle Gemming[1], and Jeffrey Kelling[1,2] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Polyalanine α-helices show strong potential for spintronic applications because of their spin-filtering ability through the Chiral-Induced Spin Selectivity (CISS) effect. To build enhanced spin-filters and understand CISS, it is important to gain better control of molecular monolayer self-assembly. This requires large scale kinetic simulations which cover the long time scales of layer formation and annealing. The kinetics of polyalanine molecules anchored to metal substrates is governed by two separate time regimes: slow diffusion on the surface and fast relaxation of the organic ensemble.

To address these challenges, we present a dual time-scale simulation approach for 2D self-assembly that combines kinetic Monte Carlo (KMC) for slow diffusion with molecular dynamics (MD) for rapid relaxation. We demonstrate a parallel implementation based on the Alpaka abstraction layer to achieve performance portability across CPUs and GPUs. This proof of concept paves the way for large-scale simulations of mono-layer self-assembly in support of future spintronic applications.

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Modeling intermolecular interactions and ordered packing in self-assembled monolayers of polyalanine α-helices — Hadis Ghodrati Saeini[1], Thi Ngoc Ha Nguyen[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 are attracting attention as promising candidates for electronic spin-filters due to the phenomenon of chiral-induced spin selectivity (CISS). This motivates substantial research to characterize the structural and electrical properties of self-assembled monolayers (SAMs) of peptide helices, for example, polyalanine (PA) α-helices. In this work, we aim to characterize the intermolecular interactions governing PA-SAM film formation. We developed an empirical potential that models the interaction between two isolated helices, derived using the density functional-based tight-binding (DFTB) method. This potential allowed us to simulate the most energetically favorable arrangements in SAM films via a Monte Carlo approach employing simulated annealing and the Metropolis algorithm. Statistical analysis of the relative positioning of adjacent molecules enabled us to classify the degree of frustration in the films. For enantiopure systems, a frustration-free arrangement was found, yielding a perfect hexagonal lattice. For mixtures of chiralities, the results showed parallel-aligned domains of differently handed helices. Both findings are in excellent agreement with experimental works.

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Spin-Dependent Transport of CISS in Polyalanine on GMR-like Au/Co/Au Interfaces — •Andreas Cordier[1], Thi Ngoc Ha Nguyen[1], Huu Thoai Ngo[1], Julian Koch[1], Lech Thomas Baczewski[2], and Christoph Tegenkamp[1] — [1]Technische Universität Chemnitz — [2]Polish Academy of Sciences, Warszawa

Chiral molecules enable the investigation of spin-selective transport in a GMR-like Au/Co/Au geometry. We studied 16-mer L-polyalanine adsorbed on such multilayers by LT-UHV-STM and STS. Topography reveals interdigitated molecular arrangements with an intermolecular spacing of ~3 nm and reduced long-range order compared to ambient conditions. STS yields a HOMO-LUMO gap of ~1.8 eV and an asymmetry of the electronic states, consistent with shifts induced by the intrinsic molecular dipole under the junction electric field. The I-V characteristics show a clear dependence on the Co magnetization orientation, evidencing CISS-driven, spin-dependent transport through the PA layer and allowing an extraction of the molecular CISS-MR.

In magnetic-field-dependent feedback measurements, the tip stabilizes at distinct equilibrium positions depending on the prior Co magnetization direction, producing a robust Δz signal that vanishes on Au/Co/Au reference samples. Using a quantitative model accounting for all resistive elements of the GMR-like stack we relate the measured Δz to the spin-dependent transmission through the molecules. In combination with forthcoming electronic-structure input, this establishes the experimental foundation for a consistent determination of the CISS-induced magnetoresistance in chiral molecules.

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Evolution of voids in molybdenum disilicide during electromigration experiments — •Julia Baldauf, Dennis Mitrenga, Tim Fink, and Philipp Kellner — CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Molybdenum disilicide (MoSi2) is used in macroscopic and microscopic heating devices.

The widespread use of MoSi2 is caused by its melting point of 2030°C and its combability with CMOS processes. Because of the high melting point MoSi2 has been considered immune to electromigration phenomena. In reality electromigration is one of the main causes of chip failure for microheaters employing MoSi2 at temperatures of 600°C up to 900°C.

Artificially generated voids were made by using a gallium based focused ion beam, are approximately circular in shape and located near the center of a line under test made of MoSi2. We employed a laser scanning microscopy technique to observe changes of the shape of artificially generated voids. Slight changes in the shape of the voids and the formation of hillocks on the rim of the voids have been observed.

Because of the low volume of the migrated material the chemical analysis remains challenging.

Machine learning is used to determine the effective ion charges used in Finite-Element-Methode-simulations of a digital twin. The digital twin will be used in conjunction with the experimental data to evaluate the effective ion charge determined by employing the machine learning algorithm.

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Towards Study of Charge Transport Mechanisms Across Grain Boundaries in Organic Monolayer Films via Near-Field Photocurrent Spectroscopy — •Jian Xiao, Francesca Falorsi, Lukas Renn, and Thomas Weitz — Georg-August-University Göttingen, Göttingen, Germany

Organic semiconductors, particularly emerging organic thin films (OTFs) comprising one to several molecular layers, enable diverse nanoscale (opto-)electronic devices. Device performance critically depends on the crystalline order within OTFs, where grain boundaries (GBs) between dissimilarly oriented domains are widely recognized as limiting factors for charge transport. While previous studies have identified two GB types, barriers and valleys, distinguished by whether their lowest unoccupied molecular orbitals (LUMOs) lie above or below those of bulk grains, the detailed transport mechanisms across these interfaces remain poorly understood.

We will report our current efforts to develop scanning near-field optical microscopy (SNOM) to investigate excited photocurrents across GBs in organic monolayer films under illumination with photon energies comparable to the energy differences between GBs and bulk grains. Our approach aims to elucidate charge transport pathways across GBs and their contribution to macroscopic current formation. We further examine how GB type and the magnitude of interfacial energy differences influence transport mechanisms. These insights may inform charge transport studies across barriers in other optoelectronic material systems.

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Superconducting diode effect in in epitaxial thin films of elemental superconductors — •Shanshan Guo[1], Nikolai Peshcherenko[1], Changjiang Yi[1], Ning Mao[1], Heda Zhang[1], Heiko Reith[2], Walter Schnelle[1], Edouard Lesne[1], Kornelius Nielsch[2], Yang Zhang[3], and Claudia Felser[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — [2]Leibnitz IFW Dresden, Dresden, Germany — [3]Department of Physics and Astronomy, University of Tennessee, Knoxville, USA

The superconducting diode effect allows for nonreciprocal, dissipationless electronic transport. It has the potential to enhance transfer current efficiency compared to the traditional semiconducting equivalent and hence have a significant impact on the design of future electronic devices. While the field is fast evolving, there are still many unanswered questions about the underlying mechanisms and origin of the phenomenon. Here we investigate the superconducting diode effect in epitaxial thin films of elemental superconductors (V, Nb and Ta). We probe its supercurrent nonreciprocity as a function of magnetic field and temperature and discuss the role spin-orbital-coupling strength plays in the superconducting diode effect in a combined simple material/device structure. Our work should stimulate the refinement of theoretical models and enable a deeper understanding of the supercurrent rectification effect.

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Cavity-modified electron mobility in monolayer black phosphorus from first principles — •Qinyan Yi[1], I-Te Lu[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Initiative for Computational Catalysis, The Flatiron Institute, Simons Foundation, New York City, NY 10010, United States of America

Cavity materials engineering offers a new route to control material properties through quantum fluctuations, without requiring external driving fields such as laser pulses. However, theoretical studies of cavity-modified transport in realistic materials are still lacking. In this work, we perform an ab initio study of monolayer black phosphorus coupled to cavity photons using quantum electrodynamical density functional theory (QEDFT), which includes an additional electron-photon exchange potential in the Kohn-Sham Hamiltonian. Our results show that cavity photons can modify the electron-phonon interaction of black phosphorus and decrease the phonon-limited scattering rate, leading to an increase in electron mobility by about 10% for a realistic coupling ratio of mode strength to bare photon frequency of 0.1, which is the upper limit of a realistic device. These results demonstrate that cavity materials engineering can modify the materials transport, highlighting its promise as a practical, non-intrusive approach for tuning material properties.