Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls H3 and H14; Poster P1)

Invited Talks

DS 4.1	Tue	9:30–10:00	H3	**Graphene-based epitaxial 2D heterosystems: making graphene great again** — •Christoph Tegenkamp
DS 7.1	Wed	9:30–10:00	H14	**Enhancing Organic Spin Valves Through Spinterface Engineering** — •Shuaishuai Ding, Wenping Hu
DS 9.1	Thu	9:30–10:00	H3	**Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces** — •Sebastian Heidenreich, Nando Hegemann, Victor Soltwisch, Markus Bär
DS 9.2	Thu	10:00–10:30	H3	**Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces** — •Bernd Bodermann, Matthias Wurm, Manuela Schiek, Jana Grundmann, Tim Käseberg
DS 12.1	Thu	16:15–16:45	H3	**Probing the Electronic Structure of Halide Perovskites** — •Selina Olthof
DS 12.2	Thu	16:45–17:15	H3	**Quantum Science with Single Atoms and Molecules on Surfaces** — •Philip Willke
DS 12.3	Thu	17:30–18:00	H3	**Gallium Nitride Technology - the second pillar of microelectronics** — •Andreas Waag
DS 12.4	Thu	18:00–18:30	H3	**Ultrafast X-ray photoelectron spectroscopy and photoelectron diffraction** — •Philip Hofmann
DS 15.1	Fri	9:30–10:00	H3	**Structure formation and growth at the metal-organic interface** — •Peter Zeppenfeld

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Sessions

DS 1.1–1.10	Mon	9:30–12:30	H3	**Thin Film Properties**
DS 2.1–2.5	Mon	9:30–10:45	H14	**Layer Deposition**
DS 3.1–3.10	Mon	15:00–17:45	H3	**2D Materials and their Heterostructures I (joint session DS/HL)**
DS 4.1–4.11	Tue	9:30–13:00	H3	**2D Materials and their Heterostructures II (joint session DS/HL)**
DS 5.1–5.5	Tue	14:00–15:15	H3	**Thin Oxides and Oxide Layers**
DS 6.1–6.8	Wed	9:30–11:45	H3	**Thin Film Application**
DS 7.1–7.7	Wed	9:30–11:45	H14	**Spins in Molecular Systems: Strategies and Effects of Hyperpolarization**
DS 8.1–8.4	Wed	12:00–13:00	H3	**Optical Analysis of Thin Films I**
DS 9.1–9.9	Thu	9:30–12:45	H3	**Optical Analysis of Thin Films II**
DS 10.1–10.4	Thu	11:30–12:30	H14	**Transport Properties**
DS 11.1–11.4	Thu	15:00–16:00	H3	**Thermoelectric and Phase Change Materials**
DS 12.1–12.4	Thu	16:15–18:30	H3	**Gaede-Jubiläumssitzung**
DS 13.1–13.64	Thu	18:00–20:00	P1	**Poster**
DS 14	Thu	18:30–20:00	H3	**Members' Assembly**
DS 15.1–15.7	Fri	9:30–11:45	H3	**Organic Thin Films, Organic-Inorganic Interfaces**

Members' Assembly of the Thin Films Division

Thursday 18:30–20:00 H3

- Report of activities in 2024
- Election of deputy speaker DS

DS 1: Thin Film Properties

Time: Monday 9:30–12:30 Location: H3

DS 1.1 Mon 9:30 H3

From ferromagnetic semiconductor to anti-ferromagnetic metal in epitaxial CrxTey monolayers — •Naina Kushwaha[1,2], Olivia Armitage[1], Brendan Edwards[1], Liam Trzaska[1], Jennifer Rigden[2], Peter Bencok[3], Deepnarayan Biswas[3], Tien-Lin Lee[3], Charlotte Sanders[2], Gerrit van der Laan[3], Peter Wahl[1,4], Phil D. C. King[1], and Akhil Rajan[1] — [1]University of St Andrews, UK — [2]Central Laser Facility, UK — [3]Diamond Light Source, UK — [4]Physikalisches Institut, University of Bonn , Germany

Two-dimensional (2D) materials can exhibit markedly distinct electronic and magnetic properties compared to their bulk counterparts [1]. Among these, the Cr-Te compounds are of particular interest. 1T-CrTe2, in particular, is a room-temperature ferromagnet in the bulk, but is only metastable, readily decomposing into self-intercalated compounds like Cr2Te3 [2]. Utilizing a nucleation-assisted molecular-beam epitaxy growth method [3], we achieve the growth of phase selective monolayer Cr2Te3 and 1T-CrTe2 with enhanced growth rates and uniformity. Characterization using X-ray magnetic circular dichroism, scanning tunneling microscopy, and angle-resolved photoemission spectroscopy reveals metallic antiferromagnetic behavior in 1T-CrTe2 and semiconducting ferromagnetic properties in Cr2Te3. These findings advance new understanding of the magnetic order in Cr-Te monolayers, and demonstrate routes to control this, of potential future interest for advancing 2D spintronics [1].

[1]Gibertini, et al., Nat. Nanotech. (2019), [2]Lasek, et al., ACS Nano (2020), [3]Rajan, et al. Adv. Mater. (2024).

DS 1.2 Mon 9:45 H3

In-situ and operando characterization of atomic layer deposited SnO_2 and SnO_2/CeO_2 heterostructures for gas sensing applications — •Rudi Tschammer, Carlos Morales, Karsten Henkel, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology, Cottbus, Germany

The amorphous and defective nature of atomic layer deposited (ALD) thin films results in material properties deviating from those of well-ordered and crystalline samples. For instance, we recently reported that ALD cerium oxide (CeO_2) ultrathin (<10nm) layers could be reduced under H_2/O_2 mixtures at room temperature without decoration with noble metals, thus opening the door to design miniaturized resistive sensors based on ALD-CeO_2 active layers. However, the remaining challenges include high electrical resistance (GΩ) and relatively long response and recovery times, which may be solved by combination with conductive oxides. In particular, tin oxide (SnO_2) has been shown to improve the sensing properties of CeO_2, tentatively explained by interface effects. Here, we present in-situ X-ray photoelectron spectroscopy (XPS) and operando spectroscopic ellipsometry measurements of ultrathin ALD-SnO_2 layers, highlighting a linear growth rate, an evolution of the Sn Auger parameter related to distinct chemical envioroments rather than different oxidation states, and changes in C and N residues with the ALD number of cycles. Lastly, preliminary results from structural and chemical characterization, as well as sensing capabilities, of ALD-SnO_2/CeO_x heterostructures are discussed.

DS 1.3 Mon 10:00 H3

RF sputtered growth of β-Ga_2O_3 on Ru(0001) films — •Aman Baunthiyal, Marco Schowalter, Martin Williams, Jon-Olaf Krisponeit, Thorsten Mehrtens, Alexander Karg, Andreas Rosenauer, Martin Eickhoff, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Gallium oxide (Ga_2O_3) is a leading candidate for high-power, high-frequency electronics due to its wide bandgap and high breakdown voltage. While its growth on insulating substrates like AlN and Al_2O_3 has been well-studied, research on metal substrates remains limited. This study investigates RF-sputtered growth of Ga_2O_3 thin films on Ru(0001) surfaces with varying roughness at temperatures from room temperature (RT) up to 600°C [1].

AFM measurements showed that surface roughness peaks at intermediate growth temperatures, then decrease at 600°C, suggesting a shift toward two-dimensional growth or increased surface diffusion. XRD revealed the amorphous nature of RT-grown Ga_2O_3 films but polycrystallinity in higher-temperature grown films. Films grown at 600°C exhibited minimal change on annealing due to pre-existing polycrystallinity. TEM confirms polycrystalline β-Ga_2O_3, with crystallite sizes of ≈ 10 nm for RT samples and ≈ 80 nm for samples grown at 600°C after annealing. These results highlight the impact of substrate morphology, growth temperature, and annealing on optimizing Ga_2O_3 films, supporting developments in Ga_2O_3-based vertical devices.

[1] Baunthiyal *et al.*, Appl. Phys. Lett. **123**, 213504 (2023).

DS 1.4 Mon 10:15 H3

Molecule adsorption at Sc(x)Ga(1-x)N surfaces investigated by photo electron 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

ScGaN can occur in various crystal orientations. The most important are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition between these orientations can be found. ScGaN surfaces with different scandium concentrations and orientations were grown by molecular beam epitaxy (MBE) to investigate the near-surface electronic structure. The interaction of gas molecules (oxygen and water) in vacuum were analyzed by X-ray (XPS) and ultraviolet photoelectron spectroscopy (UPS).

session break

DS 1.5 Mon 10:45 H3

Low temperature solid state dewetting of gold thin films on polystyrene nano structures — •Felix Lohmeyer and Jörg K.N. Lindner — Universität Paderborn, Department Physik, Warburgerstraße 100, 33098 Paderborn

Solid-state dewetting describes the breakup of a thin film into isolated objects due to surface energy minimization below the material's melting point. While well-studied for hard substrates, little research has been done on the dewetting of metal thin films on polymer substrates. This study shows that gold thin films can undergo dewetting at temperatures that preserve the underlying polymer substrate, with dewetting kinetics increasing with annealing temperature. Gold thin films (7 nm) were deposited on planar and nanostructured polystyrene (PS) substrates and thermally annealed at 100 to 120 °C, near the polymer's glass transition temperature ($T_{g,PS}$=100°C). Homogeneous spin coated PS films and nanostructured PS lamellae, created via block copolymer self-assembly, served as substrates. Dewetting was characterized using SEM, AFM, and TEM. On planar PS, dewetting was observed at any temperature and proceeded without incubation time, triggered by the initial non-uniformity of the gold film. On nanostructured PS, gold formed nanorods aligned with the polymer lamellae, breaking into particles while preserving the substrate pattern. These findings demonstrate the role of substrate morphology and temperature in dewetting and suggest a route to fabricating sub-10 nm gold structures for applications in sensing, catalysis, and nanoelectronics using BCP-based polymer templates.

DS 1.6 Mon 11:00 H3

Morphological characterization of Sub-10 nm surface patterns created by block-copolymer self-assembly — •Harikrishnan Venugopal, Janna X. Friebel, Julius Bürger, and Jörg K.N. Lindner — Universität Paderborn, Department Physik, Warburgerstraße 100

The microphase separation in block copolymers (BCPs) is a self-assembly process allowing to create ordered patterns on large substrate surfaces in short times and at low costs. Numerous applications of such patterns have been identified in the area of micro- and optoelectronics, data storage, catalysis, nanoporous membranes, and biomedical materials. If BCP self-assembly is used to create lithographic masks by removing one of the polymers selectively, for any targeted application it is important to characterise the morphology of polymer domains precisely at each processing step. In this work, we report on the morphology of silicon oxide nano structures fabricated by BCP self-assembly on Si substrates. A polystyrene-polydimethylsiloxane block copolymer (PS-b-PDMS) with a molar mass of 15 kg/mol and a PS volume fraction of 68.75 % was dissolved and spin coated onto silicon substrate. Microphase separation was initiated by solvent vapor annealing and results in the formation of fingerprint like surface patterns. A high-power oxygen plasma treatment is done to selectively remove the PS domains while converting the PDMS to silicon oxide. TEM, SEM and AFM analyses were performed to understand why after the plasma treatment half-cylinder patterns are observed.

DS 1.7 Mon 11:15 H3

Sub-10 nm Nanostructures in Thin Films of a Cylinder-Forming PS-b-PDMS Block Copolymer — •Janna X. Friebel, Harikrishnan Venugopal, Julius Bürger, and Jörg K. N. Lindner — Universität Paderborn, Germany

Block copolymers (BCPs) with a combined Flory-Huggins parameter χN > 10 form ordered domains even at low degrees of polymerization (N), enabling sub-10 nm nanostructures suitable for e.g. nanomasks in microelectronics. However, interfacial energy effects in thin films complicate the direct application of the bulk phase diagram by Bates et al. [1].

This study investigates the morphology of thin PS-b-PDMS high-χ BCP films with $N_B/N_A \approx 0.25$, spin-coated onto silicon, titanium, and chromium substrates (all with their native oxides). The films were top coated with PVA, solvent vapor annealed, PVA stripped, and the PS phase was selectively etched. Cross-sectional TEM reveals hemispherical structures instead of the expected hexagonal arrangement of cylinders, as suspected from SEM and AFM investigation. The energetic reasons for this geometry are discussed.

[1] F. S. Bates et al., Physics Today 52 (1999) 32-38.

session break

DS 1.8 Mon 11:45 H3

Ultrathin-Film Y6 at Air-Water Interface via the Langmuir-Blodgett Technique for Optoelectronic Application — •Yisak Tsegazab Gerase[1,2] and Martin Presselt[1,2] — [1]Institute of Physical Chemistry, Jena, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

Supramolecular structures are critical to the optoelectronic properties of films. The Langmuir-Blodgett (LB) technique provides precise molecular assembly, enabling control and homogenization of the morphology of Y6 Langmuir films, which is essential for scalable fabrication and commercial production. Y6, a non-fullerene acceptor, has significantly improved the power conversion efficiency of organic solar cells. We monitored the in-situ formation of Y6 Langmuir films using Brewster angle microscopy, surface pressure isotherms, and fluorescence spectroscopy. Isotherms revealed high packing densities, while compression-expansion cycles showed increased stiffness due to intermolecular rearrangements. BAM images confirmed smooth, well-defined quasi-2D films, and in-situ fluorescence spectroscopy identified the existence of Y6 fluorophore at the air-water interface and with lateral compression growth in supramolecular structure were observed. In agreement with in-situ observations, these well-ordered morphologies were further characterized after deposition on solid supports. Y6 films used in organic thin-film transistors showed a mobility of about 0.007 cm2 /Vs as cast film, comparable to other deposition techniques.

DS 1.9 Mon 12:00 H3

Femtosecond Laser Ablation (fs-LA) - A New Approach to XPS Depth Profiling — •samir mammadov — Thermo Fisher Scientific, 1 The Feldbridge Centre, Imberhorne Lane, East Grinstead, West Sussex, RH19 1XP, UK

XPS depth profiling is a widely employed analytical technique to determine the chemical composition of thin films, coatings and multilayered structures, due to its ease of quantification, good sensitivity and chemical state information. Since the introduction of XPS as a surface analytical technique more than 50 years ago, depth profiles have been performed using ion beam sputtering. However, many organic and inorganic materials suffer from ion beam damage, resulting in incorrect chemical compositions to be recorded during the depth profile. This problem has been resolved for most polymers by using argon gas cluster ion beams (GCIBs), but the use of GCIBs does not solve the issue for inorganics. A prototype XPS depth profiling instrument has been constructed that employs a femtosecond laser rather than an ion beam for XPS depth profiling purposes. This novel technique has shown the capability of eradicating chemical damage during XPS depth profiling for all initial inorganic, compound semiconductor and organic materials examined. The technique is also capable of profiling to much greater depths (several 10s microns) and is much faster than traditional ion beam sputter depth profiling. fs-LA XPS depth profile results will be shown for selected thin films, coatings, multilayers and oxidised surfaces and the outlook for this new technique discussed.

DS 1.10 Mon 12:15 H3

Optimizing erbium luminescence for integrated photonics via ytterbium co-doping and thermal annealing — •Sören Lerner[1], Felix Mania[1], Jiale Sun[2], Zheru Qiu[2], Xinru Ji[2], Yang Liu[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 ions are promising candidates for enabling efficient optical amplification of signals in photonic integrated circuits, but their practicality is hindered by insufficient output power. To address this, we utilize ion implantation into ultralow-loss silicon nitride (Si_3N_4) thin films and investigate co-doping with ytterbium ions to enhance absorption and emission through resonant energy transfer. We systematically investigate the effects of doping concentration and subsequent thermal annealing parameters using photoluminescence measurements. These findings provide insights into optimizing erbium-based light emitters for integrated photonics.

DS 2: Layer Deposition

Time: Monday 9:30–10:45 Location: H14

DS 2.1 Mon 9:30 H14

Bidirectional Growth of Functional Oxides by Molecular Beam Epitaxy — •Nicolas Bonmassar[1], Georg Christiani[2], and Gennady Logvenov[2] — [1]University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Here I present some recent results on the use of offcut substrates by enabling atomic precision layer-by-layer growth in both in-plane and out-of-plane directions. This is achieved by in situ monitoring of the oscillations of the reflected high-energy electron diffraction (RHEED) patterns. The potential of this method is demonstrated using a bidirectionally grown superlattice of alternating $LaMnO_3$ and $SrMnO_3$ layers, showing interfacial ferromagnetism. This superlattice serves as a model system to showcase the method's versatility through detailed structural and functional characterization by using various scanning transmission electron microscopy techniques, sheet resistance measurements, and magnetometry. Next, the approach is applied to the growth of superconducting $La_{1.84}Sr_{0.16}CuO_4$ thin films grown in ozone atmosphere on various offcut substrates, where the anisotropic critical current is found to arise from two distinct mechanisms induced by the substrate geometry.

Furthermore, I will present the issues we faced when we first started this project and how we had overcome well-known problems like the loss over the in situ RHEED oscillations, terrace broadening, step bunching, 3D defect formation and the concomitant loss of functionalities like superconductivity.

DS 2.2 Mon 9:45 H14

Enabling vacuum process monitoring with time-of-flight spectroscopy — •Marco John, Kristian Kirsch, Andreas Trützschler, Christoph Bartlitz, Marcel Herrmann, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, Großlöbichau, Germany

A crucial aspect to manage industrial vacuum processes is the importance of fast in-situ monitoring and control of process parameters such as pressure and residual gas composition. Improving process control in this way minimizes production errors, avoids damage to process equipment and ensures longer operating times. The capabilities of hot cathodes and quadrupole mass spectrometers are limited for this complex task, as they can only measure either the total pressure or the gas composition. One answer to this challenge is our novel ion source NOVION*, which combines the well-known technology of time-of-flight spectroscopy with our patented ion trap to an industrially available gas analyzing application.

In this talk we present the fundamental physical principles of the novel ion source and explain the compact combination of time-of-flight spectroscopy with our own patented ion trap. We discuss the advantages and limits in different applications as well as best practices in the field and show the capability to push the principle to its limits at high pressures without compromising the performance or lifetime of the filaments.

DS 2.3 Mon 10:00 H14

Selective Area Atomic Layer Deposition via Photoexcitation — •Paul Butler[1,2], Stefan A. Maier[3], and Ian D. Sharp[1,2] — [1]Walter Schottky Institut, Technische Universität München, 85748, Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technical Universität München, 85748, Garching, Germany — [3]School of Physics and Astronomy, Monash University, 3800, Melbourne, Australia

While atomic layer deposition (ALD) is a powerful technique for uniformly coating complex surfaces with thin films, achieving lateral control of ALD layers remains a primary challenge. In this work, we examine a selective-area ALD (S-ALD) process via photoexcitation of the growth surface. We demonstrate that optical laser excitation enhances ALD-growth of TiO$_2$ films on gold surfaces deposited onto Si and SiO$_2$. These surfaces were exposed to titanium isopropoxide (TTIP) and ozone as reactants for the ALD process, during which some of the samples were exposed to laser illumination. In-situ ellipsometry was used to monitor the growth rate of the TiO$_2$ films during ALD, and ex-situ ellipsometry was used to map the height profile of the resulting TiO$_2$ films deposited. The results show intensity-dependent enhanced growth on surfaces that were excited with laser illumination. We also show that a shadow mask can be used to make patterned depositions.

DS 2.4 Mon 10:15 H14

Enabling FAIR Data Practices in MBE Growth and Characterization — •Andrea Albino[1], Hampus Näsström[1], Sarthak Kapoor[1], Altuğ Yildirim[2], Oliver Bierwagen[2], Martin Albrecht[3], and Sebastian Brückner[1,3] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Data-driven materials science is transforming materials design by moving beyond traditional trial-and-error methods. Molecular beam epitaxy (MBE) experiments highlight the challenge of navigating complex parameter spaces [1], often exceeding human cognitive limits, particularly when integrating diverse datasets. This complexity is compounded by the absence of standardized models for capturing detailed experimental workflows and instrument diversity. Addressing these issues requires metadata aligned with FAIR (Findable, Accessible, Interoperable, Reusable) principles [2].

Within the NOMAD ecosystem (nomad-lab.eu) [3], we digitize the data lifecycle for MBE growth, including in-situ and ex-situ characterization. Key tools, like Electronic Laboratory Notebooks (ELNs), systematically document growth procedures, enabling streamlined data management and AI-driven analytics to optimize MBE processes.

[1] O. Bierwagen et al., J. Phys. Condens. Matter 28, 22 (2016) [2] M. Wilkinson et al., Sci. Data 3, 160018 (2016) [3] M. Scheidgen et al., J. Open Source Software 8, 5388 (2023)

DS 2.5 Mon 10:30 H14

Role of point defects on the superconducting transition temperature in NbTIN thin films with positron annihilation spectroscopy — •Sebastian Klug[1], Maik Butterling[1], Maciej Oskar Liedke[1], Eric Hirschmann[1], Andreas Wagner[1], Bharath Reddy Lakki Reddy Venkata[2], Aleksandr Zubtsovskii[2], and Xin Jiang[2] — [1]Institute of Radiation Physics, HZDR, Germany — [2]Chair of Surface and Materials Technology, University of Siegen, Germany

Positron annihilation spectroscopy (PAS) is a non-destructive method for studying point defects in materials with high sensitivity. It can sense defect densities in the range of 10^{15} to $10^{19} cm^{-3}$. The time for positrons to annihilate with electrons depends on the local electron density. Therefore, positrons can be trapped in neutral and negatively charged open-volume defects. Positrons are implanted into the studied material with a defined implantation energy. Changing of this energy allows for depth-resolved characterization. The user facility ELBE of HZDR provides the two main PAS techniques Doppler broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS) which allows for evaluation of the atomic environment of defects as well as defect size and density.

In this contribution the most recent results of magnetron sputtered NbTiN thin films as promising candidate for improving the characteristics of superconducting radio-frequency cavities (SRF cavities) will be discussed. The correlation between defect size and their concentration and the superconducting transition temperature will be highlighted.

DS 3: 2D Materials and their Heterostructures I (joint session DS/HL)

Time: Monday 15:00–17:45 Location: H3

DS 3.1 Mon 15:00 H3

Nanoscale NMR of two-dimensional solids using NV centers in diamond — •Marcel Martin[1], Mokessh Kannah Ciwan[1], Yejin Lee[2], Jakob Nachtigal[1], Nicola Poccia[3,4], Uri Vool[2], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [4]Department of Physics, University of Naples Federico II, Naples, Italy

Nuclear magnetic resonance (NMR) is a powerful method to investigate electronic properties of condensed matter but is inherently limited by its low sensitivity. Nitrogen-vacancy (NV) centers in diamond are quantum sensors that allow extending NMR to thin films and μm-scale exfoliated flakes of 2D materials which exhibit electronic phases such as charge density waves (CDW) and superconductivity. For the latter, NMR is especially powerful as it can elucidate the pairing symmetry of the charge carriers.

In this talk, we first discuss solid-state nano-NMR with NV centers of CaF$_2$, a testbed material for this method. The ultimate goal, however, is to study the CDW and Ising superconductivity phases of few-layer NbSe2 with nano-NMR. In this context, we present initial optical studies of NbSe$_2$ flakes which have been exfoliated and transferred onto a diamond. In addition to this, we will present results of conventional NMR on bulk NbSe$_2$ which serve as a reference.

DS 3.2 Mon 15:15 H3

Twist-tunable spin control in twisted bilayer bismuthene — •Ludovica Zullo[1,2,3,4], Domenico Ninno[4,5], and Giovanni Cantele[5] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France — [4]Dipartimento di Fisica E. Pancini, Università degli Studi di Napoli *Federico II*, Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy — [5]CNR-SPIN, c/o Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy

The role of spin-orbit coupling (SOC) in twisted bilayers has gained increasing attention due to its potential for spintronics, opening a quest for new layers with substantial SOC. In this work [1], by means of first principles calculations, we investigate how the interplay between SOC and twist angle impacts the band structure and spin textures of twisted bilayer bismuthene. We find that the twist angle can be deemed a control knob to switch from a small-gap semiconductor to a metallic behavior. Most crucially, the accurate analysis of the energy bands close to Fermi energy reveals a twist-tunable splitting in the mexican-hat shape of the bands that can otherwise be obtained only by applying enormous electric fields, providing insight into innovative technologies for future spintronic devices. [1] Ludovica Zullo, Domenico Ninno, Giovanni Cantele, Phys. Rev. B, 110, 165411 (2024)

DS 3.3 Mon 15:30 H3

Iron Diffusion in Thermally Stable $Ti_3C_2Cl_2$ MXenes under UHV Conditions — •Moritz Vanselow[1], Maksim Riabov[2], Hanna Pazniak[2], Thierry Ouisse[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

MXenes are 2D materials derived from a MAX phase precursor. Molten salt etching of $Ti_3C_2Cl_2$ results in hydrophobic $Ti_3C_2T_X$ MXenes with T_X = -Cl as a termination species [1]. $Ti_3C_2Cl_2$ MXenes are deposited on Si(100)/SiO_2 and we in situ study its chemical stability by mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum. Compared with standard hydrophilic $Ti_3C_2T_X$ MXenes, where T_X = -F, =O, and -OH, fluorine and hydroxyl groups can be removed by annealing at temperatures up to 1000 K, the thermal stability of $Ti_3C_2Cl_2$ MXenes is significantly enhanced. Moreover, intercalated water changing the MXene sheet separation, is not present in hydrophobic $Ti_3C_2Cl_2$ as proven by ex situ X-ray diffraction, wide-angle X-ray scattering (WAXS) and X-ray photoelectron spectroscopy (XPS). After optimizing the annealing procedure, we in situ intercalate Fe by e-beam assisted deposition on top of MXene thin films and subsequent Fe diffusion by soft annealing at 600 K. This work is funded by a joint ANR-DFG-Project under ANR-23-CE09-0031-01 and DFG ID 530103526. [1] T. Zhang et al., Chem. Mater. 36, 1998 (2024).

DS 3.4 Mon 15:45 H3

Interactions Between Two-Dimensional Crystals and Molecules via Density Functional Theory — •Stefan Wolff[1], Xin Chen[2], Tobias Dierke[1], and Janina Maultzsch[1] — [1]Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

The unique properties of two-dimensional (2D) materials can be modified through chemical functionalization, driven by their interactions with functional groups or molecules. Density functional theory (DFT) calculations are employed to investigate non-covalent functionalization of bilayer graphene with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) molecules. The interactions between the graphene layers and the HATCN molecules play a significant role in determining the functionalization behavior, which depends on the stacking arrangement. Locally stacked regions within the moiré lattice of twisted bilayer graphene (tBLG) play a crucial role for functionalization. Consequently, the moiré pattern of tBLG can serve as a template to control the degree of functionalization. Furthermore, laser-triggered covalent functionalization of molybdenum disulfide (MoS_2) enables the fabrication of patterned 2D heterostructures with phenyl-based interface linkers. Through DFT calculations, various potential binding motifs and their associated optical properties are predicted. Calculations of reaction energies and Raman modes provide insights into the likelihood of different reaction pathways and the structures they yield.

DS 3.5 Mon 16:00 H3

Toward high-sensitivity and low-power consumption gas sensor devices based on 2D-transistors. — •Aurelio García Valenzuela[1], Zahra Fekri[1], Madhuri Chennur[1], Nikol Lambeva[1], Jens Zscharschuch[1], Victoria Constance Köst[2], Krysztof Nieweglowski[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Electronic Packaging Technology, AVT, TU-Dresden, Germany

Two-dimensional (2D) materials exhibit excellent properties compared to their bulk counterparts and are promising for applications like gas sensors. Their high surface-to-volume ratio and surface-active sites enhance gas absorption and sensitivity, addressing challenges in detecting low concentrations and reducing power consumption.

This work presents the fabrication and testing of 2D materials-based field-effect transistor (FET) gas sensors. Mechanically exfoliated 2D materials are stacked into heterostructures to create back-gated FETs, with device patterning achieved via electron beam lithography.

The devices were exposed to NH3 and NO2 gases at various temperatures. Gas interactions caused systematic changes in p- and n-type currents and shifts in the transfer curve, depending on gas concentration and type (donor or acceptor). These results demonstrate the suitability of 2D materials-based FETs as efficient and sensitive gas sensors.

short break

DS 3.6 Mon 16:30 H3

Pressure-dependent Effective Hamiltonian and Topological Transitions for Twisted Bilayer Transition Metal Dichalcogenides — •Miftah Hadi Syahputra Anfa[1], Sabri Elatresh[1,2], Hocine Bahlouli[1,3], and Michael Vogl[1,2] — [1]Physics Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia — [2]Interdisciplinary Research Center (IRC) for Intelligent Secure Systems, KFUPM, Dhahran, Saudi Arabia — [3]Interdisciplinary Research Center (IRC) for Advanced Materials, KFUPM, Dhahran, Saudi Arabia

Recent studies have shown the existence of nontrivial topological moire bands in twisted bilayer transition metal dichalcogenides (TMDs), which depend on the twist angle. Motivated by this, we present a study of such a system under applied vertical pressure. The study begins by first considering the untwisted bilayer case without pressure. We find that the system can be described by an effective low-energy Hamiltonian that behaves approximately quadratic and includes layer-shift dependent terms that we were able to determine by symmetry. The structure is then relaxed under pressure in the 0.0 - 3.5 GPa range using ab initio density functional theory (DFT). The DFT band structures for each corresponding pressure are fitted to the effective Hamiltonian to obtain the pressure-dependent parameters. Consecutively, the explicit expression for the twisted pressure-dependent Hamiltonian is obtained by treating the twist as a position-dependent shift between layers. We then present changes in Chern number results for the important energy bands due to pressure.

DS 3.7 Mon 16:45 H3

Effect of spin-dependent tunneling in a $MoSe_2/Cr_2Ge_2Te_6$ van der Waals heterostructure on exciton and trion emission — •Annika Bergmann[1], Swarup Deb[1,2], Veronika Schneidt[1], Mustafa Hemaid[1], Kenji Watanabe[3], Takashi Taniguchi[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, Rostock University, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]Research Center for Electronic and Optical Materials, Tsukuba, Japan — [4]Research Center for Materials Nanoarchitectonics, Tsukuba, Japan

In recent years, thin films of magnetic van der Waals materials have gained increasing interest due to their potential applications in spintronics. For instance, heterostructures (HS) consisting of ferromagnetic CRI_3 and a WSe_2 monolayer have demonstrated the existence of magnetic proximity effects, manifesting in the lifting of WSe_2 valley degeneracy as well as helicity-dependent photoluminescence (PL) emission of the WSe_2 monolayer in proximity to the 2D ferromagnet [1,2]. Here, we study HS consisting of monolayer $MoSe_2$ and few-layer ferromagnetic $Cr_2Ge_2Te_6$ (CGT). Under circularly polarized excitation, PL measurements show that the $MoSe_2$ exciton-trion emission ratio depends on the relative orientation of excitation helicity and CGT magnetization, even though the PL emission itself is unpolarized. This hints at an ultrafast, spin-dependent interlayer charge transfer that competes with exciton and trion formation and recombination.

[1] D. Zhong et al., Science Advances, 3 (2017)

[2] D. Zhong et al., Nat. Nanotechnol. 15 (2020)

DS 3.8 Mon 17:00 H3

Magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Tauqir Shinwari[1], Kacho I. A. Khan[1], Jens Herfort[1], Michael Hanke[1], Chen Chen[2], Joan M. Redwing[2], Achim Trampert[1], Mehak Loyal[3], Gerhard Jakob[3], Mathias Kläui[3], Roman Engel-Herbert[1], and João Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]2D Crystal Consortium Materials Innovation Platform, Materials Research Institute, The Pennsylvania State University, PA, United States — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

Van der Waals (vdW) heterostructures consisting of two-dimensional (2D) ferromagnetic and nonmagnetic materials hold great promises for tailoring their magnetic and transport properties. Here we report on the magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2$ (FGT, with x ≈ 0.2)/WSe_2 heterostructures tailored via the FGT thickness. Magnetic characterizations and anomalous Hall effect measurements with both out-of-plane and in-plane magnetic fields reveal an enhanced perpendicular magnetic anisotropy (PMA) in thinner FGT and a ferromagnetic order up to room temperature. The pronounced unconventional Hall effect (UHE) suggests the possible formation of skyrmions. The thickness-dependent asymmetric magnetoresistance reveals a unique magnetization switching process. Our results demonstrate the high potential of all-epitaxial FGT/WSe_2 heterostructures for the advancement of future 2D spintronic applications.

DS 3.9 Mon 17:15 H3

Effect of Ni-doping on the structural/magnetic properties of large area epitaxial 2D-ferromganet Fe_3GeTe_2 — •Kacho Imtiyaz Ali Khan[1], Tauqir Shinwari[1], Hua Lv[1], Frans Munnik[2], Jens Herfort[1], Michael Hanke[1], and Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Helmholtz-Zentrum Dresden- Rossendorf e.V. Dresden, Germany

2D ferromagnets with strong perpendicular magnetic anisotropy exhibit magnetic order down to the monolayer thickness and have the potential to overcome long-term challenges faced by 3D ferromagnets to build up advanced energy-efficient spintronic devices. In this work, we show the large-area epitaxial growth of Ni-doped Fe_3GeTe_2 films via molecular beam epitaxy. X-ray diffraction measurements demonstrate high-quality epitaxy of pure Fe_3GeTe_2 phase on graphene/SiC(0001) substrates. Magneto-transport measurement unveils the ferromagnetic nature of the film, with strong perpendicular magnetic anisotropy for pure Fe_3GeTe_2 and Ni-doped films. However, the Ni-doped Fe_3GeTe_2 shows a decrease in Curie temperature T_C with an increase in Ni-doping. We believe that the Ni doping modifies the lattice parameters and structure (e.g., Ni intercalation), which results in the dilution of magnetic properties of Fe_3GeTe_2 by reducing the T_C down to 50 K. Our findings show the role of Ni incorporation on the ferromagnetic behavior of Fe_3GeTe_2 films, which is crucial for the development of future spintronic devices.

DS 3.10 Mon 17:30 H3

The epitaxial growth of Gallium Selenide — Michele Bissolo, Marco Dembecki, Florian Rauscher, Jan Schabesberger, Abhilash Uhle, Jonathan J. Finley, Gregor Koblmüller, and •Eugenio Zallo — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Garching, Germany

Group III-VI post-transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are van der Waals semiconductors with layer-dependent electronic, thermoelectric and optical properties, strong photoresponsivity, and a Caldera type valence band [1]. However, the limited scalability and risk of contamination of the standard mechanical exfoliation technique are detrimental to developing devices at an industrial scale. Here, we demonstrate the molecular beam epitaxy growth of PTMC [2] GaSe on 2-inch sapphire wafers. To study the pristine properties of this air-sensitive material in situ, we perform Raman spectroscopy in a UHV chamber directly connected to the growth chamber. Film composition and morphology are investigated by tuning the growth temperature and group VI/III flux ratio and by correlating them with the known spatial gradients across the whole substrate. The combination of these findings with ex-situ surface morphology characterization allows us to construct the phase diagram and identify the 2D layered region [3]. Perspectives on the growth of PTMC on 2D substrates and the epitaxial registry will be discussed. [1] H. Cai, et al., Appl. Phys. Rev. 6, 041312 (2019).[2] E. Zallo, et al., npj 2D Mater. & Appl. 7, 19 (2023).[3] M. Bissolo, et al., [to be submitted].

DS 4: 2D Materials and their Heterostructures II (joint session DS/HL)

Time: Tuesday 9:30–13:00 Location: H3

Invited Talk DS 4.1 Tue 9:30 H3

Graphene-based epitaxial 2D heterosystems: making graphene great again — •Christoph Tegenkamp — Institut für Physik, TU Chemnitz

2D materials and their heterostructures are at the forefront of research, anticipated to serve as fundamental building blocks for new quantum materials. Proximity coupling is a key concept in this domain, enabling diverse and novel functionalities. Epitaxial graphene (EG) grown on SiC(0001) resembles a truly 2D electron gas system, celebrated for its manifold and flexible functionalization schemes at both its vacuum and interface sites. These functionalization strategies enable extreme doping scenarios in graphene, tuning spin-orbit coupling, realizing interface states, or introducing mini-bands through zone folding. The controlled transition from linear to flat bands in EG, along with the coupling of functionalized epitaxial graphene to 2D electron gases (2DEGs), opens avenues for exploring electronic correlation effects and mesoscopic phenomena in epitaxial 2D heterostructures. In this presentation, I will showcase some recent findings achieved through the adsorption and intercalation of elements such as Pb and Sn, demonstrating their potential to further tune the properties of graphene.

DS 4.2 Tue 10:00 H3

Proximity-induced spin-orbit coupling in bilayer graphene quantum wires — •Michael Laumer and Angelika Knothe — Universität Regensburg, 93053 Regensburg, Germany

The gate-tuneable band gap and the possibility to tailor its band structure by proximitizing with other 2D materials [1] make bilayer graphene (BLG) an excellent platform for future quantum technologies. By applying spatially modulated displacement fields, one may confine BLG's charge carriers into electrostatically induced nanostructures [2, 3]. Proximitizing the BLG with a transition metal dichalcogenide (TMDC) strongly enhances the SOC of the adjoining graphene layer [1]. Fascinated by the concept of proximity-tailoring BLG nanostructures, we convey the idea of proximity-inducing SOC to a gate-confined BLG quantum wire. We theoretically study the resulting quantized subband structure for different SOC strengths and as a function of the wire geometry. Our results help us understand how proximity-induced SOC manifests in confined geometries and identify different regimes of the wires' electronic properties.

[1] K. Zollner, M. Gmitra, and J. Fabian. Swapping exchange and spin-orbit coupling in 2d van der waals heterostructures. Phys. Rev. Lett., 125:196402, (2020). [2] A. Knothe and V. Fal'ko. Influence of minivalleys and berry curvature on electrostatically induced quantum wires in gapped bilayer graphene. Phys. Rev. B, 98:155435, (2018). [3] H. Overweg et al. Topologically nontrivial valley states in bilayer graphene quantum point contacts. Phys. Rev. Lett., 121:257702, (2018).

DS 4.3 Tue 10:15 H3

Above room temperature ferromagnetism in large-area Fe_3GaTe_2/graphene van der Waals heterostructures — •Tauqir Shinwari[1], Kacho Imtiyaz Ali Khan[1], Hua Lv[1], Atekelta Abebe Kassa[1], Frans Munnik[2], Achim Trampert[1], Michael Hanke[1], Jens Herfort[1], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V. Dresden, Germany

Two-dimensional (2D) magnetic materials and van der Waals (vdW) heterostructures offer new possibilities for the realization of advanced spintronic devices. Fe_3GaTe_2, a 2D ferromagnetic metal with a high Curie temperature ($\sim$ 360K) and strong perpendicular magnetic anisotropy, has emerged as a promising candidate for energy-efficient magnetic devices. However, all investigations conducted in Fe_3GaTe_2 so far have been performed using millimeter-sized bulk crystals and flakes exfoliated from them, both not suitable for integration in device processing. Hence, it is crucial to develop controlled large-scale growth of this material and investigate its properties. In this contribution, we present a breakthrough in the high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films on epitaxial graphene/SiC(0001) substrates using molecular beam epitaxy. These results are highly relevant for the future development of high-performance spintronic devices based on 2D heterostructures potentially revolutionizing data storage, processing, and quantum computing applications.

DS 4.4 Tue 10:30 H3

Modeling carbon nanomembranes through molecular dynamics simulations — •Levin Mihlan and Jürgen Schnack — University of Bielefeld

Carbon nanomembranes (CNMs) are nanometer-thin materials syn-

thesized via electron-induced crosslinking of aromatic self-assembled monolayers. CNMs can be functionalized for various applications, initially serving as molecular filters. Due to their presumed irregular internal structure, these membranes pose challenges for standard spectroscopic efforts, often being insufficiently informative [1]. Ehrens et al. initially conducted molecular dynamics simulations to investigate CNM formation, replicating crosslinking and pore formation via momentum transfers in carbon-only systems [2]. Here, we extend the approach by incorporating hydrogen atoms, which may play a critical role in the crosslinking process, even though they largely disappear in the final CNM products. This additionally reduces the number of theoretical assumptions. We examine whether and in what way pores form and analyze properties such as aromaticity, sp content, and Young's modulus to compare with previous simulations and experiments.
[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" Chem. Phys. Chem 21, 1006 (2020)
[2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416 (2021)

session break

DS 4.5 Tue 11:00 H3

Photo-electrochemical oxidation and thinning of transition metal dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Franz Gröbmeyer[2], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Walter Schottky Institute, Physics Department and TUM School of Natural Science, Technical University of Munich — [2]Nanoinstitute Munich and Faculty of Physics, Ludwig-Maximilians-Universität — [3]Naval Research Laboratory, Washington, D.C

Two-dimensional transition metal dichalcogenides (TMDs) exhibit unique optoelectronic and mechanical properties. For their integration in functional devices and for catalytic applications, it is crucial to understand and control their behavior in the reactive environments. Here, we investigate the stability of thin MoS$_2$, WS$_2$, MoSe$_2$ and WSe$_2$ films in acidic, neutral, and basic solutions using a three-electrode photoelectrochemical cell, which enables experiments under both illumination and in the dark. Under anodic conditions, sulfides and selenides undergo different protonic reactions, depending on the pH of the electrolyte, resulting in different resistances to oxidation. Additional exposure to light from a solar simulator creates photo-excited holes, which drive a self-limiting electrochemical thinning procedure that enables the top-down fabrication of large-area TMDs with a thickness of only a few layers. The degradation, initiated at the edges or defects, propagates through the flakes and can be monitored in-situ using an optical microscope. Under laser excitation, multilayer TMDs can be thinned in predefined patterns, paving a new route for processing and integration of 2D materials into functional devices.

DS 4.6 Tue 11:15 H3

Rapid MOCVD synthesis of stratified MoS2 and WS2 2D heterostructures — •Nikolas Dominik, Sebastian Klenk, Cormac Ó Coileáin, and Georg S. Duesberg — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, München, Deutschland

The two-dimensional (2D) structure of layered materials such as the transition metal dichalcogenides MoS2 and WS2, imparts exceptional electrical, mechanical and optical properties. This makes them particularly interesting for electronic, photovoltaic and sensing application. Van der Waals heterostacks, composed of assembled 2D materials, expand on the possible range of properties, and so have attracted extensive attention due to factors such as ultrafast carrier transport and high bandgap tunability.

Here we present metal-organic chemical vapour deposition (MOCVD) synthesis of MoS2/WS2 combination heterostructures using a highly controllable industrial-scale multi-precursor system, thus avoiding the laborious need for manual stacking. We show how this synthesis method allows the creation of clearly defined and highly ordered stacks by producing a 7-layer combination structure below 10 nm. We explore the characteristics of these films using Raman spectroscopy and XPS, EDX, TOF-SIMS and microscopy techniques.

DS 4.7 Tue 11:30 H3

Unveiling the mechanism of monolayer selective large-area exfoliation of 2D materials — •Jakob Ziewer[1], Abyay Ghosh[1], Michaela Hanušová[2], Luka Pirker[2], Otakar Frank[2], Matěj Velický[2], Myrta Grüning[1], and Fumin Huang[1] — [1]Queen's University Belfast, Belfast, U.K. — [2]J. Heyrovský Institute of Physical Chemistry

Metal assisted exfoliation has made it possible to selectively isolate single crystal monolayers of 2D materials at sizes up to a centimetre [1][2]. This represents a million fold increase compared to standard tape exfoliation.

In this presentation the mechanism of enhanced yield is discussed. Through spectroscopic measurements and observation of macroscopic bubbles it is discovered that the Au substrate decouples attached MoS_2 monolayers from the remaining crystal. The interfacial weakening is dependant on the thickness of the crystal and is maximised for thick crystals.

These findings are used to explain the mechanism behind metal assisted exfoliation and are expected to extend to other Au-2D heterostructures.

[1] Velický, M.; et. al. Mechanism of Gold-Assisted Exfoliation of Centimeter-Sized Transition-Metal Dichalcogenide Monolayers. ACS Nano 2018, 12, 10463*10472. [2] Huang, Y.; et. al. Universal Mechanical Exfoliation of Large-Area 2D Crystals. Nat. Commun. 2020, 11:2453.

session break

DS 4.8 Tue 12:00 H3

Probing the electronic band structure of the 2D magnetic materials MPS3 (M=Fe,Ni) across magnetic phase transitions — •Jeff Strasdas[1], Benjamin Pestka[1], Biplab Bhattacharyya[1], Adam K. Budniak[2], Marcus Liebmann[1], Niklas Leuth[1], Honey Boban[3], Lutz Waldecker[1], Bernd Beschoten[1], Christoph Stampfer[1], Lukasz Plucinski[3], Efrat Lifshitz[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH, Aachen, Germany — [2]Schulich Chem. Fac., Solid State Inst., Russell Berrie Nanotech. Inst., Helen Diller Quantum Center, Technion - Israel Inst. of Technology, Haifa, Israel — [3]Forschungszentrum Jülich, Peter Grünberg Inst. (PGI-6), Jülich, Germany

We investigate the band structure of the van der Waals materials FePS3 [1] and NiPS3, both 2D antiferromagnetic insulators, using μm-scale Angular Resolved Photoelectron Spectroscopy (ARPES), above and below their Néel temperatures (TN). The data is compared with DFT+U calculations and simplified selection rules to deduce the orbital character of changing bands. In FePS3, we observe three distinct band structure changes across TN, involving bands with Fe 3d, S 3p, and pure P 3p character, reflecting the intricate competition of direct exchange between Fe atoms and superexchange via S and P atoms. In NiPS3, we identify one band shift near Γ across TN, containing a band of mixed Ni and S character. Here, pronounced deviations from the DFT+U calculations indicate more complex electronic correlations. Moreover, we refine the photoelectron selection rules using ARPES data from CrPS4. [1] B. Pestka et al. doi:10.1021/acsnano.4c12520

DS 4.9 Tue 12:15 H3

Investigation of 1T-TaS2 phase transition and charge transfer phenomena at interfaces with perovskites — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Centre of Scientific Research Demokritos, 15341 Athens, Greece — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Athens, Greece

1T-TaS2 is a distinguished 2D-layered transition metal dichalcogenide with a rich phase diagram upon cooling including charge density wave (CDW) states and a Mott insulating phase. On the other hand, halide perovskites (HPs) are emerging as a unique class of materials in the field of photonics due to their intriguing optoelectronic properties. The combination of 1T-TaS2 with HPs is proposed as a viable solution to overcome the drawbacks of each category thanks to charge transfer phenomena.

In this work, we studied the phase transitions of 1T-TaS2 as a function of the cooling rate. In the case of nanothick crystals, CDW phase transitions were observed upon gradual cooling but they were totally absent afrer a vigorous cooling. On the contrary, for bulk crystals the CDW phase transitions were totally independent of the cooling rate. Furthermore, we developed 1T-TaS2/HPs heterostructures and we investigated charge transfer phenomena by XPS and UPS spectroscopy, both revealing electron transfer from 1T-TaS2 towards perovskite. Charge transfer could also enable the development of high-performance hybrid optoelectronic devices based on these materials.

DS 4.10 Tue 12:30 H3

The effect of a perpendicular electric field on charge-spin interconversion coefficients in proximitized graphene on 1T-TaS$_2$ monolayer — •Juraj Mnich[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

The proximity-induced spin-orbit coupling and exchange interactions in the graphene-based heterostructures provides an effective way to manipulate with charge-spin interconversion coefficients. In the talk we focused on charge-spin interconversion in bilayer and trilayer heterostructures of 1T-TaS$_2$ and graphene. By modulating the temperature, we can access the charge density wave phase and switch between the magnetic and non-magnetic phases of 1T-TaS$_2$ affecting consequently the graphene electrons. Using linear response theory we showed the dependence of charge-spin interconversion coefficients on a perpendicular applied electric field. For the specific configurations of the 1T-TaS$_2$ and graphene we observed a change in both the sign and the magnitude of the non-equilibrium spin density as a response to the perpendicular electric field. This result indicates a possibility of using electric fields as a tool to control the direction of spin density.

This work was supported by the APVV-SK-CZ-RD-21-0114 and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008.

DS 4.11 Tue 12:45 H3

Self spin-orbit torque in proximitized graphene on 1T-TaS$_2$ monolayer — •Martin Gmitra[1,4], Maedeh Rassekh[1], Juraj Mnich[1], and Marko Milivojević[2,3] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

We show that self spin-orbit torque induced in graphene-based van der Waals heterostructures represents a platform to extract the Rashba phase – a proximity-induced spin-orbit coupling parameter. Performing first-principles calculations, tight-binding modeling, and non-equilibrium Greens function transport calculations for graphene on 1T-TaS$_2$ monolayer we found that charge current in graphene generates non-equilibrium spin accumulation and self-torque in graphene due to the proximity-induced spin-orbit coupling and exchange interaction. The Rashba spin-orbit torque is a dominant contribution and weakly depends on the direction of magnetization in 1T-TaS$_2$. We propose that the magneto-optical Kerr effect can directly extract the Rashba spin-orbit coupling phase.

This work was supported by the APVV-SK-CZ-RD-21-0114, EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008, and IMPULZ IM-2021-42.

DS 5: Thin Oxides and Oxide Layers

Time: Tuesday 14:00–15:15 Location: H3

DS 5.1 Tue 14:00 H3

How to functionalize 2D states at oxide interfaces by controlled redox reaction — •Pia Maria Düring, Andreas Fuhrberg, Timo Krieg, Verena Reva, and Martina Müller — FB Physik, Universität Konstanz, 78457 Konstanz

Oxide electronics provide the key concepts and materials for enhancing silicon-based semiconductor technologies with novel functionalities. In a recent paper, we provide evidence for individually emerging hole- and electron-type 2D band dispersions at Fe-SrTiO$_3$ heterostructures [1]. The emergence of p- or n-type bands is closely linked to the Fe oxidation state which enables the possibility to tune the interface properties to set or even switch between negatively (n) charged electrons or positively (p) charged holes. One of the main processes that controls the interface properties is the oxygen exchange between the film and the substrate. Using our UHV-MBE system, we grow high-quality ultrathin TM (e.g. Fe, Co and Hf) oxide films on SrTiO$_3$ substrates by systematically varying the growth parameters, e.g. (i) growth temperature, (ii) substrate annealing, and (iii) metal film thickness. The present work discusses the effect of different growth parameters on the interfacial properties like oxygen vacancies, the oxidation state of the TM oxide as well as the concentration of defects in SrTiO$_3$, which strongly influences the valence band alignment between electron and hole band bending. In this way, we can effectively control the properties of the 2D interface to ultimately add ferroic functionalities to these confined electronic states.

[1] P. M. Düring et al., Advanced Materials, 2024, 2390217.

DS 5.2 Tue 14:15 H3

Adsorption-controlled growth of α-(Al,Ga)2O3 and β-(Al,Ga)2O3 on Al2O3 by suboxide molecular-beam epitaxy (S-MBE) — •Sushma Raghuvansy[1], Marco Schowalter[1], Alexander Karg[1], Manuel Alonso-Orts[1,2], Martin Williams[1], Stephan Figge[1], Andreas Rosenauer[1,2], Martin Eickhoff[1,2], and Patrick Vogt[1,3] — [1]Institute of Solid-State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359, Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany — [3]Max Planck Institute for solid state research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Gallium oxide (Ga2O3) is a promising ultra-wide band gap semiconductor with extremely high (predicted) breakdown field for high performance power electronics.

α-Ga2O3 is isostructural to α-Al2O3, and allows alloying over the entire composition range from Ga2O3 (x=0) and Al2O3 (x=1) in α-(AlxGa1-x)2O3 [1]. For β-(AlxGa1-x)2O3, range with which Al can be alloyed is 0 <x < 0.61, which leads to a bandgap range of 4.6-5.9 eV [2].

In this contribution, we demonstrate the growth of high quality α-(Al,Ga)2O3 on Al2O3 (10-10) and Al2O3 (11-20) and β-(Al,Ga)2O3 on Al2O3 (0001) by suboxide molecular beam epitaxy (S-MBE). We investigated the influence of Al flux and growth parameter space of (Al,Ga)2O3 alloys on differently oriented Al2O3 substrates.

[1] R. Jinno et al., Science Advances 7 (2021) [2] T. Oshima et al., Jpn. J. Appl. Phys. 48, 070202 (2009)

DS 5.3 Tue 14:30 H3

Tuning the interlayer coupling in La$_{0.7}$Sr$_{0.3}$MnO$_3$ / LaNiO$_3$ **multilayers with strong perpendicular-magnetic-anisotropy** — •Jörg Schöpf[1], Valentina Piva[1], Paul H. M. van Loosdrecht[1], Padraic Shafer[2], Divine P. Kumah[3,4], Xuanyi Zhang[3,4], Lide Yao[5], Sebastiaan van Dijken[6], and Ionela Lindfors-Vrejoiu[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, USA — [3]Department of Physics, Duke University, Durham, USA — [4]Department of Physics, North Carolina State University, Raleigh, USA — [5]OtaNano-Nanomicroscopy Center, Aalto University, Aalto, Finland — [6]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

We report on the magnetic interlayer coupling between Ru-substituted La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin films separated by few unit cell thin LaNiO$_3$ spacers, grown by pulsed-laser-deposition and investigated by SQUID-mangetometry, magnetotransport and the magneto-optive-Kerr effect. The magnetic anisotropy in Ru-substituted La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin films, in combination with light compressive strain of a LSAT substrate, allows to tune the magnetic anisotropy from easy-plain to strong perpendicular-magnetic-anisotropy. LaNiO$_3$, allows for strong FM- or AFM-coupling between the manganite layers depending on spacer thickness. We propose a layer-by-layer type magnetization reversal in the case of strong PMA, introduced by substituting 10% of Mn by Ru, while films with lower substitution of 5% and weaker PMA instead show signs of collective, spin-flop-type transitions.

DS 5.4 Tue 14:45 H3

Multinary compositionally graded, spatially addressable materials libraries by pulsed laser deposition — •Jorrit Marius Bredow, Marius Grundmann, and Holger von Wenckstern — Felix Bloch Institute for Solid State Physics, Leipzig University

The discovery of novel, functional materials is increasingly based on the investigation of multinary materials with large composition spaces. Therefore, combinatorial synthesis and high-throughput characterization methods are preferable for the discovery of functional multicomponent materials. Here, pulsed laser deposition (PLD) from segmented targets allows the synthesis of spatially addressable materials libraries (SA-ML) with continuous compositional gradients[1].

We demonstrate that PLD is a viable method for synthesizing multicomponent SA-ML using n-fold azimuthally segmented targets. We present a roadmap for the fabrication of fivefold segmented targets using MgO, CoO, NiO, CuO, and ZnO, which can be readily applied to different material combinations. Moreover, we compare two approaches to target and deposition process design for PLD of SA-ML. The composition of the SA-ML is determined by high-throughput energy dispersive X-ray spectroscopy confirming the successful synthesis of a fivefold compositionally graded SA-ML by combinatorial PLD. Aditionally, the height distributions and elemental compositions are simulated with the thickness distribution parameters of the binary oxides and the simulation results are compared to the experimental data.

[1] H. von Wenckstern, Z. Zhang, F. Schmidt, J. Lenzner, H. Hochmuth, and M. Grundmann, CrystEngComm, 15, 10020, 2013.

DS 5.5 Tue 15:00 H3

Tri-functionality in a Single Oxide Interface-Based Nanostructure with Reconfigurable Logic-in-Memory Applications — •Soumen Pradhan[1], Kirill Miller[1], Fabian Hartmann[1], Merit Spring[2], Silke Kuhn[1], Victor Lopez-Richard[3], Michael Sing[2], Ralph Claessen[2], and Sven Höfling[1] — [1]Julius-Maximilians-Universität Würzburg, Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Deutschland — [2]Julius-Maximilians-Universität Würzburg, Würzburg-Dresden Cluster of Excellence ct.qmat, Experimentelle Physik 4, Deutschland — [3]Department of Physics, Federal University of São Carlos, Brazil

We demonstrate transistor (T), memristive (M), and memcapacitive (MC) functionalities in nanowires, based on quasi-two-dimensional electron system in $LaAlO_3/SrTiO_3$ heterostructures depending on the biasing condition at lateral gates. Combining one T and one M, the device can be utilized for short term and long term synaptic plasticity. However, arranging two T in parallel and series with one M, the structures show logic OR and AND gates, respectively. In addition, the devices can memorize the logic output even after grounding the inputs taking advantage of its long term memory. Interestingly, the single structure can be reconfigured between OR and AND logic. Our findings on oxide nanostructures together with logic-in-memory and reconfigurability in logic as well as in functionality open a path towards oxide-based monolithic integrated circuits for brain inspired neuromorphic computing.

DS 6: Thin Film Application

Time: Wednesday 9:30–11:45 Location: H3

DS 6.1 Wed 9:30 H3

Fluorescent SiON-Doped Si Thin Films in Miniature Temperature Sensor Fabrication Using Machine and Deep Learning with Low Root Mean Square Error — Ali Karatutlu[1], Timuçin Emre Tabaru[2], •Zehra Gizem Mutlay[1], Esra Kendir Tekgül[1], Nurhan Güneş[2], and Bülend Ortaç[1] — [1]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University, Ankara, Türkiye — [2]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, Sivas, Turkey

SiON-doped Si, discovered by our project team last year (DOI: Advanced Optical Materials, 2023, DOI: 10.1002/adom.20230009), has a special molecular matrix with a refractive index that can be controlled depending on the amount of SiON. The counterpart structures, such as SixNy, SiOxNy, or Si-rich Si3N4, are conventional structures with general properties such as mechanical durability, thermal stability, chemical resistance, electrical insulation, and optical transparency. We report that SiON-doped Si can have a relatively even higher refractive index from 2.07 to 2.56 near the telecom wavelength of 1310 nm, depending on the SiON content. In terms of application, SiON-doped Si thin films were tested at room temperature to 200°C using different packaging materials such as borosilicate glass and aluminum, and their use as miniature temperature sensors will be demonstrated. The preliminary temperature-fluorescence spectrum correlation was investigated using machine learning and deep learning methods that yield the root mean square error of this system to be as low as 2°C.

DS 6.2 Wed 9:45 H3

Electron-transparent free-standing ultrathin membranes for studying gas-solid and liquid-solid interfaces at high pressures — •Max Gertig[1], Carlos Morales[1], Andreas Schubert[2], Carlos Alvarado[2], Christian Wenger[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]IHP Leibniz-Insitut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The chemical reactions of heterogenously catalyzed processes take place at the gas-solid and liquid-solid interfaces. Thus, significant efforts have been dedicated to developing new methods to study them under realistic conditions. In recent years, electron-transparent graphene windows have been used in ambient pressure X-ray photoelectron spectroscopy (AP-XPS) to separate liquids and gases at ambient pressure from a high vacuum. Following this design, we present free-standing ultrathin (up to 10 nm) Al_2O_3 membranes fabricated by atomic layer deposition (ALD) which are electron-transparent to tender and hard X-rays. Three different commercial supports are used: TEM SiN perforated membranes (1 μm), single-hole stainless steal apertures (20 μm), and TEM Cu-grids (80 μm). Their conformity has been examined by scanning electron microscopy (SEM) and atomic force microscopy (AFM), whereas their chemical composition and homogeneity by energy dispersive X-ray (EDX) mapping. Additionally, confocal μ-Raman microscopy complements the chemical and structural characterization. Conventional free-standing graphene membranes have also been fabricated for comparison purposes.

DS 6.3 Wed 10:00 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. Preliminary work in the literature suggests that the phase transition temperature of the anatase to rutile structural phase transition of TiO_2 is lowered for by alloying Cu. However, that the band gap of $Cu_xTi_{1-x}O_2$ decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates by conventional rf-sputtering employing a TiO_2 ceramic target and Cu wires as Cu source. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

DS 6.4 Wed 10:15 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

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decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Furthermore, we find that the morphology of the $Cu_xTi_{1-x}O_2$ thin films changes with increasing x. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

session break

DS 6.5 Wed 10:45 H3

Achieving superconductivity in infinite-layer nickelate thin films by aluminum sputtering deposition — •dongxin zhang[1], A. Raji[2], L. M. Vicente-Arche[1], A. Gloter[2], M. Bibes[1], and L. Iglesias[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, 91405, France — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, 91405, France

After decades of research, the recent discovery of superconductivity in hole doped infinite-layer nickelates (ABO2) has offered new perspectives to deepen the understanding of high-temperature superconductivity. infinite-layer (IL) nickelates are synthesized by topotactic reduction that selectively removes all apical oxygens of the precursor perovskite ABO3 phase. This is typically achieved by an ex-situ complex annealing using CaH2 as a reducing agent. However, the progress in this field is hampered by significant challenges in materials synthesis and the limited number of research groups capable of producing high-quality superconducting (SC) samples.Here, we present a new method to synthesize SC IL nickelates Pr0.8Sr0.2NiO2 thin films using an aluminum overlayer deposited by sputtering as a reducing agent. We optimized the aluminum deposition conditions and achieved SC samples reduced either in-situ or ex-situ. In-situ Al reduction enhances the quality of the SC Pr0.8Sr0.2NiO2 films, with a maximum transition temperature Tconset of 17 K. This simplified synthesis approach, more accessible than existing ones, enables more research groups to produce high-quality SC nickelate samples, Possibly advancing experimental understanding of superconductivity in IL nickelate.

DS 6.6 Wed 11:00 H3

Deposition and characterisation of NbTiN thin films for application in SRF cavities — •Bharath Reddy Lakki Reddy Venkata, Aleksandr Zubtsovskii, and Xin Jiang — Chair of Surface and Materials Technology, University of Siegen, Germany

Superconducting radio frequency (SRF) cavities are key components for modern particle accelerators. While bulk niobium (Nb), with the highest lower critical magnetic field, Hc1 (0.18 T), and transition temperature, Tc (9.23 K), among elemental superconductors, has dominated SRF applications, the performance of bulk Nb cavities has reached theoretical limits. Recent research focuses on the use of superconducting thin films of Nb or other alternative higher Tc materials, such as NbN, NbTiN, Nb3Sn, MgB2, etc, to enhance SRF cavity performance and cost efficiency. However, their lower Hc1 limits high accelerating gradients and quality factors. Gurevich's SIS multilayer theory offers a breakthrough to shield an underlying superconductor from the applied magnetic fields, thus increasing the maximum accelerating gradient beyond the bulk Nb limits. This study investigates NbTiN thin films deposited on Si substrates using reactive DC- and HiPIMS techniques. Deposition parameters were optimised to achieve improved microstructure and superconducting properties, enabling their integration into SIS structures. To understand the microstructural characteristics of NbTiN films, positron annihilation spectroscopy (PAS) was employed alongside SEM, XRD, AFM, and EDX, offering deeper insights into how deposition techniques and parameters affect material performance.

DS 6.7 Wed 11:15 H3

T-dependent switching of molecular spin-crossover (SCO) monolayers — •Fabian Streller[1], Kirill Gubanov[1], Stephen Goodner[2], Marat Khusniyarov[2], and Rainer Fink[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich Alexander Universität Erlangen Nürnberg — [2]Lehrstuhl für Anorganische und Allgemeine Chemie, Friedrich Alexander Universität Erlangen Nürnberg

Spin-crossover (SCO) complexes are regarded as promising materials in spintronics, molecular electronics and ultra-high-density memory systems applications. Switching between diamagnetic low-spin (LS) and paramagnetic high-spin (HS) species is triggered by external stimuli, e.g., change of temperature, pressure, or illumination with light.[1] One major challenge is the transfer from solution or bulk towards thin films or even monolayers on well-defined surfaces without quenching of the switching behaviour. Six-coordinate iron(II) complexes have been used as SCO materials. This material is attached to the surface via a bidental phenanthroline ligand containing moieties suitable for bonding to the substrate. We report on a step-by-step formation of SCO-active single-layer films on Au(111) surfaces. Thus created specimens were characterized by atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and temperature dependent near edge x-ray absorption fine structure (NEXAFS) to follow the molecular switching. Research is funded by the BMBF (contract 05K22WE2) [1] B. Rösner, M. Milek, A. Witt, B. Gobaut, P. Torelli, R. H. Fink, M. M. Khusniyarov Angewandte Chemie. 2015, 127, 13168-13172.

DS 6.8 Wed 11:30 H3

High Accuracy Reflection Prediction Model for Multi-Layer Anti-Reflection Coatings Using Deep Learning and Machine Learning — •Iremnur Duru, Semih Oktay, and Timuçin Emre Tabaru — Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey

In order to optimize the thickness parameters, this work employs Machine Learning (ML) and Deep Learning (DL) approaches to develop an accurate reflection prediction model that will direct the design of filters with multilayer Anti-Reflection Coating (ARC). A dataset of information derived from 3000 (1500 Ge- Al2O3, 1500 Ge- SiO2) computer simulations based on the thicknesses of multilayer structural materials has been used to create this model. Al2O3 and SiO2 served as the second layers in both coatings, with Ge serving as the substrate. Reflectance values for wavelengths ranging between the 3-5 *m and 8-12 *m bands characteristic of the mid-wave infrared (MWIR) and long-wave infrared (LWIR) bands are included in the data set. The average reflectance in the given 2-layer data set was at least 0.36 at thicknesses of 515 nm Ge and 910 nm SiO2. In terms of predicting reflectance values, the results demonstrate that machine learning (ML) models*specifically, decision tree, random forest and bagging methods perform better than the DL model and offer a useful guide for conceptualizing and manufacturing optical thin-film filters.

DS 7: Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Time: Wednesday 9:30–11:45 Location: H14

Invited Talk DS 7.1 Wed 9:30 H14

Enhancing Organic Spin Valves Through Spinterface Engineering — •Shuaishuai Ding and Wenping Hu — Institute of Molecular Aggregation Science, School of Science, Tianjin University, Tianjin, China

Organic spin valves hold immense promise for efficient spintronic devices, driving advancements in information processing and storage technologies. The spinterface, the interface between an organic semiconductor and a ferromagnetic electrode, plays a crucial role in the performance of these devices. However, the inherent instability of the spinterface poses challenges that must be addressed to fully realize this potential. To tackle these issues, we have developed a comprehensive approach that combines innovative fabrication techniques and material engineering. Electrode transfer technology enhances interfacial properties by enabling the precise deposition of high-quality ferromagnetic electrodes onto organic semiconductors, while doping with F4-TCNQ effectively improves spin injection efficiency through modulation of electronic and magnetic characteristics. Moreover, the engineering of controllable bottom spinterfaces allows for precise regulation of spin injection, resulting in highly tunable device performance. By leveraging the spinterface, we have achieved in-situ control of device tunability, significantly expanding the multilevel resistance modulation of organic spin valves. These advancements not only address key challenges of unstable spinterface but also establish novel methods for device modulation, marking an important leap forward in organic spintronics.

DS 7.2 Wed 10:00 H14

Hyperpolarised electron spins as a sensitive probe for investigating structure–function relationship in organic energy materials — •Till Biskup — Universität Rostock, Rostock, Germany

Energy conversion and storage is of paramount importance, and organic functional materials are increasingly being used for this purpose. Hyperpolarised electron spins as created, e.g., by light excitation act as sensitive probe of their environment. This allows to investigate the structure–function relationship of these materials by using time-resolved electron paramagnetic resonance (TREPR) spectroscopy. Insights range from morphology and details of the aggregation behaviour in both, film and solution to triplet routes to the electronic structure of these materials far beyond exciton delocalisation. Here, we focus particularly on the effects of conjugation break and systematic backbone variation on exciton delocalisation as well as solvent and cooling rate on aggregate formation. TREPR spectroscopy provides insight into these effects with molecular resolution that is not available by and complementary to other methods.

DS 7.3 Wed 10:15 H14

The CISS magnetoresistance effect for polyalanine and polyproline molecules studied by ambient STM — •Thi Ngoc Ha Nguyen[1], Lech Tomasz Baczewski[2], Tobias Theiss[3], Tanja Gulder[3], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Ger- many — [2]Reichenhainerstr., 70 — [3]Institute of Organic Chemistry, Faculty of Chemistry and Mineralogy, Leipzig University, Leipzig, Germany

The chirality induced spin selectivity (CISS) effect has been up to now measured in a wide variety of systems but its exact mechanism is still under debate. Whether the spin polarization occurs at an interface layer or builds up in the helical molecule is yet not clear. We investigated the current transmission through helical polyalanine molecules, revealing a strong and length dependent dipole moment, as a part of a tunnel junction realized with a scanning tunneling microscope. Depending on whether the molecules were chemisorbed directly on the magnetic Au/Co/Au substrate or at the STM Au-tip, the magnetizations of the Co layer had been oriented in the opposite direction in order to preserve the symmetry of the IV-curves. These results show that besides the helicity also the electric dipole play a crucial role. Latest experiments with polyproline with a small electric dipole moment showed that the CISS effect is almost vanishing. Our results can be explained by a spin-polarized or spin-selective interface effect, induced and defined by the helicity and electric dipole orientation of the molecule at the interface.

session break

DS 7.4 Wed 10:45 H14

Analysis of polaron pair lifetime dynamics and secondary processes in exciplex driven TADF OLEDs using organic magnetic field effects (MFE) — •Annika Morgenstern[1], Dominik Weber[2], Lukas Hertling[1,3], Konstantin Gabel[1], Ulrich T. Schwarz[1], Daniel Schondelmaier[2], Dietrich R.T. Zahn[1,3], and Georgeta Salvan[1,3] — [1]Institute of Physics, TU Chemnitz — [2]Physical Engineering and Computer Science, WH Zwickau — [3]MAIN, TU Chemnitz, Chemnitz

MFE in TADF materials have been shown to influence the reverse intersystem crossing and to impact on electroluminescence and conductivity. Here, we present a novel model combining Cole-Cole and Lorentzian functions to describe low and high MFE originating from hyperfine coupling, the Δg mechanism, and triplet processes. We applied this approach to organic light-emitting devices of third generation based on TCTA and TPBi, exhibiting blue emission, to unravel their loss mechanisms. The quality of the regression function was evaluated using k-fold cross-validation. The scoring was compared to various alternative fitting functions, which were previously proposed in literature. Density functional theory calculations, photoluminescence, and electroluminescence studies validated the formation of a TADF exciplex system. Furthermore, we propose successful encapsulation using a semi-permeable polymer, showing promising results for magnetic field sensing applications. This study provides insights into the origin of MFE in exciplex-TADF materials, with potential applications in optoelectronic devices and sensing technologies.

DS 7.5 Wed 11:00 H14

Employing CISS for Modification of Skyrmion Diffusion and Size — •Fabian Kammerbauer[1], Yael Kapon[2], Theo Balland[1], Shira Yochelis[2], Yossi Paltiel[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

Chirality-induced spin selectivity (CISS) is a phenomenon that has garnered significant attention due to its ability to generate large spin polarizations in organic molecules and its associated effects, such as the magnetic switching of ferromagnets induced by chiral molecules [1]. In hybrid systems, these chiral molecules have been found to influence magnetic properties, including changes in the magnetization [2]. This study explores the interaction between chiral molecules, specifically alpha-helix polyalanine, and chiral spin structures such as magnetic skyrmions. The skyrmions are stabilized in ferromagnetic/heavy metal multilayers via the Dzyaloshinskii-Moriya interaction [3]. Through magneto-optic Kerr effect imaging, we demonstrate that chiral polypeptides can alter the stability of skyrmions by shifting the temperature and magnetic field ranges where they remain stable. Furthermore, we reveal the impact of chiral molecules on skyrmion size and thermal skyrmion diffusion.

[1] R. Naaman et al. Nat. Rev. Chem. 3, 250 (2019)
[2] Y. Kapon et al. J. Chem. Phys. 159, 064701 (2023)
[3] K. Everschor-Sitte et al. J. Appl. Phys. 124, 240901 (2018)

DS 7.6 Wed 11:15 H14

Microscopic and Macroscopic CISS Effect Characterization: Moving from MBE to Sputter-Deposited Au/Co/Au Substrates — •Lokesh Rasabathina[1], Thi Ngoc Ha Nguyen[1], Julia Krone[1], Annika Morgenstern[1], Franziska Schölzel[1,2], Markus Gössler[1], Karin Leistner[1], Aleksandr Kazimir[4], Jannik Knoche[4], Christina Lamers[4], Irene Coin[4], Lech Thomasz Baczewski[5], Christoph Tegenkamp[1], Georgeta Salvan[1,2], and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology,Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Leipzig University, Leipzig, Germany — [5]Polish Academy of Sciences, Warszawa, Poland.

Adsorption of alpha-helical polyalanine molecules on metallic substrates enables interfacial selective electron transport with a defined spin direction, a phenomenon known as Chirality Induced Spin Selectivity (CISS). We combine microscopic STM/STS of hybrid spin-valve structures with macroscopic MOKE magnetometry for CISS effect characterization on Au/Co/Au substrates. Microscopically we observe magneto resistance changes across the hybrid spin-valve structure and macroscopically we find a coercivity enhancement of the Co layer after exposure to molecules. To use more complex systems, we moved from MBE to sputterd substrates and discuss the challenges related to this transition.

DS 7.7 Wed 11:30 H14

Towards a quantum sensing approach to single-cell chemical and mechanical analysis using nanoscale NMR — •Baha Sakar[1], Sirswa Kuldeep Shree Ram[1], Maximilian Püllmann[1], Frank Sauer[2], Rustem Valiullin[1], Josef A. Käs[2], and Nabeel Aslam[1] — [1]Felix-Bloch-Institut für Festkörperphysik - Universität Leipzig, Leipzig, Deutschland — [2]Peter-Debye-Institut für Physik der weichen Materie - Universität Leipzig, Leipzig, Deutschland

Understanding single-cell mechanical and chemical properties is key to exploring cellular behavior and dysfunction, influencing processes like development, immune response, and disease progression, including cancer metastasis. While fluorescence microscopy enables structural insights and tracking, it lacks the chemical specificity of conventional NMR. The latter is however limited to ensemble measurements and cannot resolve single-cells. In this study, we utilize a quantum sensing platform based on NV centers in diamond, which are atomic-scale spin defects capable of detecting nuclear spins with sensitivities up to fifteen orders of magnitude higher than conventional NMR, enabling single-cell resolution. By applying resonant microwave pulse sequences and specially designed magnetic fields, we probe the NMR signal of the cells' nuclear spins. In this talk, we will discuss the steps towards studying the micromechanical and chemical properties of single cells, distinguishing between intracellular and extracellular molecular diffusion processes. Furthermore, we will present initial results of correlating fluorescence microscopy and NMR spectroscopy with the goal to investigate the link between cell mechanics and tumor aggressiveness.

DS 8: Optical Analysis of Thin Films I

Time: Wednesday 12:00–13:00 Location: H3

DS 8.1 Wed 12:00 H3

Initial stages of Palladium growth on vicinal Si(001)-(2*1) surfaces — •Sandhya Chandola[1], Norbert H. Nickel[1], Julian Plaickner[2], Jörg Rappich[1], Karsten Hinrichs[1], and Norbert Esser[2] — [1]Nanoscale Solid-Liquid Interfaces, Helmholtz-Zentrum Berlin für Materialien und Energie,Schwarzschildstr. 8, 12489 Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Although palladium-based silicides are of great interest in many microelectronic applications, their formation mechanisms are still not fully understood, especially for thin films where the silicidation reaction may be controlled from the initial Pd-Si interactions at the interface.

The early stages of palladium silicide formation have been investigated in ultra-high vacuum (UHV), using Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy on vicinal Si(001) surfaces with different degrees of ordering. Raman spectroscopy has identified silicide-like reacted phases at the Si-Pd interface upon annealing, with the appearance of several phonon modes which are in very good agreement with vibrational modes obtained from ab initio calculations for Pd incorporation into Si surface layers.

The growth morphology of the Pd-Si structures was shown to be dependent on the initial surface reconstruction with in-situ RAS and ex-situ AFM (atomic force microscopy) clearly distinguishing between two types of structures depending on the substrate template.

DS 8.2 Wed 12:15 H3

Ultrafast Charge Carrier Dynamics in Niobium Probed in the Visible Spectral Range — •Noah Stiehm[1], Shirly Espinoza[2], Mateusz Rebarz[2], Saul Vazquez Miranda[2], Erik Müller[3], Hannes Töpfer[3], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany — [2]ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 25241 Dolní Břežany, Czech-Republic — [3]Technische Universität Ilmenau, Fachgebiet Theoretische Elektrotechnik, Helmholtzplatz 2, 98693 Ilmenau, Germany

With the recently developed experimental method of femtosecond time-resolved spectroscopic ellipsometry (trSE) [1], it is possible to obtain the transient dielectric function of a sample after excitation in a pump-probe scheme. We present results of applying the technique to study the ultrafast charge carrier dynamics in the transition metal Niobium. We show that it is possible to observe bleaching in the dielectric function for several 100 picoseconds and up to 1 nanosecond, depending on the pump wavelength, resulting from exciting charge carriers into higher conduction bands, where they relax into band minima and remain stable for some time until recombination.

The initial results from this study at room temperature provide valuable insight into the ultrafast charge carrier dynamics and good motivation to conduct further investigations under cryogenic conditions in the superconducting phase.

[1] S. Richter *et al.*, Rev. Sci. Instrum. 92, 033104 (2021).

DS 8.3 Wed 12:30 H3

Investigation of metal surfaces using Surface Resonant Raman Scattering — •Sarang Bhasme, Mariella Denk, Simon Kalteis, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

We have recently demonstrated the possibility to investigate surface phonons on metals by surface resonant Raman spectroscopy (SRRS), in which the Raman cross section is significantly enhanced by resonant excitation of optical transitions involving surface electronic states [1]. Here we report new investigations regarding the phonon and electron scattering mechanism on clean and adsorbate-modified Cu(110) surfaces using SRRS and reflectance difference spectroscopy (RDS) under ultra-high vacuum (UHV) conditions and variable temperatures. We have modified the Cu(110) surface electronic states via ion bombardment and by adsorption of small molecules such as oxygen or CO to explore its effect on the Raman signals. We find that both the phonon and the electron related scattering strongly depend on the details of the surface cleanliness and structural properties, underscoring the influence of the surface electronic structure and adsorbate interactions on the Raman signatures.

[1] M. Denk et al., Phys. Rev. Lett. 128, 216101 (2022).

DS 8.4 Wed 12:45 H3

Watching hydrogen diffusion into Lutetium and Yttrium thin films with Pd cap layers — •Zahra Hojjati, Philipp Flad, and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

Hydrogenated Lutetium is one of the materials that may have a potential to be used as high-temperature superconductor under high pressure. Recently, reports have indicated that the Lu-H-N system undergoes a phase transition to blue when hydrogenated, with unconfirmed reports suggesting superconductivity. Therefore, we investigate hydrogen-lutetium interactions and the dynamics of hydrogen diffusion within lutetium, which is influenced by the ambient temperature, crystal structure and the hydrogen concentration. Hydrogen diffusion in metals involves interstitial diffusion through the lattice and surface absorption. We find that lutetium is a good hydrogen storage material due to its diffusion properties.

We analyzed the progression of the blue hydrogenation front in Lutetium and subsequently measured the drift velocity for each sample. We calculated the activation energy required for protons to overcome the potential barrier using the Arrhenius equation. Following this, we determined the diffusion constant based on the diffusion equation. We also carry out the same experiments with Yttrium.

DS 9: Optical Analysis of Thin Films II

Time: Thursday 9:30–12:45 Location: H3

Invited Talk DS 9.1 Thu 9:30 H3

Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces — •Sebastian Heidenreich[1], Nando Hegemann[1], Victor Soltwisch[2], and Markus Bär[1] — [1]Mathematical Modelling and Data Analysis, PTB, Abbestr. 2-12, 10587 Berlin — [2]Radiometry with Synchrotron Radiation, PTB, Abbestr. 2-12, 10587 Berlin

For the analysis of thin films and nanostructured surfaces, indirect optical measurement techniques are often used to determine the optical and geometrical properties by solving an inverse problem. Due to measurement errors and model errors, the results are subjected to uncertainties. In the talk we give an overview about statistical inverse problems with applications in the metrology of thin films and nanostructured surfaces. We start with a discussion of the advantages and disadvantages of frequently used Least-Squares, then consider the Maximum-Likelihood method and introduce the Bayesian approach as a statistical method [1]. We apply the Bayesian approach to thin film examples as well as to line grating structures and show how to deal with measurement uncertainties and model errors. Furthermore, we discuss some drawbacks of the Bayesian method and present recent developments like polynomial chaos, transport maps or neural networks to tackle these drawbacks [2]. –[1] Soltwisch, Fernandez Herrero, Pflüger, Haase, Probst, Laubis, Krumrey, Scholze, J. Appl. Cryst. 50, 2017; Heidenreich, Gross, Bär, Metrologia 55(6), 2018. [2] Hegemann, Heidenreich, J. Open Software 8 (89), 2023; Hagemann, Hertrich, Casfor, Heidenreich, Steidl, Mach. Learn:Sci. Technol. 5, 2024.

Invited Talk DS 9.2 Thu 10:00 H3

Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces — •Bernd Bodermann[1], Matthias Wurm[1], Manuela Schiek[2], Jana Grundmann[1], and Tim Käseberg[1] — [1]Optical Nanometrology, PTB, Bundesallee 100, 38116 Braunschweig — [2]Center for Surface and Nano-Analytics (ZONA) Johannes Kepler University Linz, Austria

Spectroscopic Mueller ellipsometry is a widely used method for analysing thin films and nanostructured surfaces. The extension to imaging ellipsometry enables measurements on small measurement objects << 1 mm2 and investigations of local parameter variations. However, as an integral and indirect measurement method, the determination of the corresponding measurement uncertainties is challenging and requires complex analysis methods. Imaging ellipsometry, involves an even higher level of complexity both in terms of data analysis and the necessary metrological system characterisation. We give an overview of various experimental sources of uncertainty including structure-induced contributions and how these can be characterised. Both deterministic and stochastic contributions of the measurement system as well as the samples under test will be discussed. Additionally, we present investigations of sensitivity-enhanced ellipsometry, by e.g. exploiting local plasmonic or dielectric resonances in the sample structure, and advanced methods that use additional structures to amplify and/or guide resonances for the detection and characterisation of periodic and non-periodic structures.

session break

DS 9.3 Thu 10:45 H3

Structured Light Microscopy for Optical and Topological Characterization — •Denis Ukolov, Polina Gromova, and Peter Lemmens — IPKM, TU-BS, Braunschweig, Germany

Structured light beams with orbital angular momentum (OAM) are applied to study topological properties of thin films and metasurfaces. Using a laser confocal microscope with integrated interferometry, we investigate phase distributions and topological features of chiral structures.

Experimental data are compared with simulations to understand the interaction of OAM with surface geometry and its topological effects. This method offers a novel approach to characterizing surface properties in complex systems.

Work supported by DFG EXC-2123 QuantumFrontiers - Light and Matter 390837967.

DS 9.4 Thu 11:00 H3

Synchrotron-based VUV ellipsometry on passivated Si samples for optical thin film metrology — •Julian Plaickner[1], Alexander Gottwald[2], Mattia Mulazzi[2], Jörg Rappich[3], Karsten Hinrichs[3], Christoph Cobet[4], Johanna Reck[5], and Norbert Esser[1] — [1]Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [3]Nanoscale Solid-Liquid Interfaces, Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Albert Einstein Str. 15, 12489 Berlin — [4]Center for Surface and Nanoanalytics, Johannes Kepler Universität, Altenbergerstr. 69, 4040 Linz — [5]SENTECH Instruments GmbH, Schwarzschildstr. 2, 12489 Berlin

The vacuum ultraviolet (VUV) spectral range spectral range is characterized by a lack of reliable data on optical properties due to the extreme surface sensitivity and the requirements of a high brightness light source. A method for determining traceble optical data with well-defined uncertainty budget is tested on novel reference materials. For this purpose, chemically passivated vicinal silicon surfaces were measured between 2 and 30 eV with the synchrotron-based VUV ellipsometer[1] at the Metrology Light Source (MLS) of the PTB. X-ray photoelectron spectroscopy (XPS) and IR ellipsometry measurements serve as quality cross checks for the prepared surfaces. In the spectral range between 2 and 6 eV, results are compared to reference measurements made with commercial SENTECH ellipsometers.

DS 9.5 Thu 11:15 H3

Tailoring Properties of Epitaxially Grown Bismuth Telluride Thin Films through Stoichiometric Control — •Felix Hoff, Christoph Ringkamp, Alexander Kiehn, Thomas Schmidt, Dasol Kim, Jonathan Frank, Timo Veslin, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

The Earth's crust contains a significant number of minerals formed by elements such as Bi and Te, which is surprising given their scarcity. This rich mineral diversity can be attributed to strong interlayer interactions within layered chalcogenides, leading to complex phase diagrams. Bismuth tellurides, in particular, exhibit various stacking sequences that influence their properties as thermoelectrics and topological insulators. While their structural and thermoelectric properties are well-studied in bulk forms, high-quality thin films and their optical and vibrational properties remain underexplored. We address this gap by examining the vibrational and dielectric properties of epitaxially grown thin films of nine distinct BiTe compositions grown on Si (111). Using Raman and fs pump-probe spectroscopy, we characterized the lattice dynamics while optical spectroscopy was employed to determine the dielectric properties. The variation in phonon frequencies with respect to the Bi share can be attributed to the differing strengths of the interlayer bonds. The height of the dielectric absorption peak increases with increasing Bi share, accompanied by a shift in the absorption maximum to lower photon energies. Our results demonstrate the potential of the BiTe system as a versatile and tunable platform for thin film applications.

DS 9.6 Thu 11:30 H3

VUV ellipsometry for the determination of thin film optical constants — •Mattia Mulazzi[1], Julian Plaickner[2], Jörg Rappich[3], Alexander Gottwald[1], and Norbert Esser[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587, Berlin, Germany — [2]Technische Universität Berlin, Hardenbergstr. 36, 10623, Berlin, Germany — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Motivated by the purpose of determining the optical constants of thin films materials, we present our investigation method based on spectroscopic ellipsometry in the vacuum-ultraviolet spectral range using monochromatised synchrotron radiation. The measurements are characterised by low noise and high accuracy, both quantified according to state-of-the-art metrological procedures, and are well-suited to be fit by numerical methods to obtain the refractive index and the absorption coefficient in a non-parametric way, i.e., independent of the underlying physics of the material under investigation. We show exemplary measurements on surfaces of hydrogen-passivated Si, native SiO2 on Si, graphene on Si and the evaluation steps necessary to determine the optical constants from the measured data.

session break

DS 9.7 Thu 12:00 H3

Optical absorption by two-dimensional excitons (with and without screening) — •Stefan Zollner and Carlos Armenta — New Mexico State University, Las Cruces, NM

Two-dimensional excitons form not only in 2D layered materials (such as transition metal dichalcogenides) or in quantum wells. They also dominate the visible absorption by 2D van Hove singularities in 3D semiconductors. As an example, we measured and calculated the optical absorption of germanium near the E_1 and $E_1 + \Delta_1$ transitions. The 2D character of these transitions stems from the large optical mass along the (111) direction, where the highest valence bands and the lowest conduction band are nearly parallel. Elliot's formalism for the Sommerfeld enhancement of optical absorption (as modified by Tanguy for 2D excitons) provides an excellent description of these absorption peaks, if the momentum matrix element from $\vec{k} \cdot \vec{p}$-theory is used as the optical dipole matrix element. We also discuss how band filling with Fermi-Dirac statistics after intense laser excitation reduces the absorption. We are not aware of a (Banyai-Koch) theory that can be applied to the screening of 2D excitons. This work was supported by the US Air Force (FA-9550-24-1-0061).

DS 9.8 Thu 12:15 H3

All-optical quality-control of indenene intercalation into graphene/SiC — •Cedric Schmitt[1,2], Simone Sotgiu[3], Stefan Enzner[2,4], Jonas Erhardt[1,2], Elena Stellino[3], Domenico Di Sante[5], Giorgio Sangiovanni[2,3], Ralph Claessen[1,2], Simon Moser[1,2], and Leonetta Baldassarre[3] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Department of Physics, Sapienza University of Rome — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [5]Department of Physics and Astronomy, University of Bologna

Intercalating two-dimensional quantum materials beneath a sheet of graphene provides effective environmental protection and facilitates ex situ device fabrication. However, developing a functional device requires rapid, large-scale screening methods to evaluate the quality of the intercalant, which to date can be monitored only by slow, UHV-based surface science techniques. In this study, we utilize ex situ Raman micro-spectroscopy to optically and non-destructively identify the quantum spin Hall insulator indenene, a monolayer of indium sandwiched between a SiC(0001) substrate and a single sheet of graphene. Color modulation combined with indenene's distinctive low-frequency Raman fingerprint enables rapid assessment of its homogeneity and crystalline quality. Density functional perturbation theory indicates that this Raman signature originates mainly from indenene's shear and breathing modes, while additional higher-order modes are tentatively attributed to defect-assisted and two-phonon Raman processes.

DS 9.9 Thu 12:30 H3

Moiré lattice of twisted bilayer graphene as template for non-covalent functionalization — •Tobias Dierke[1], Stefan Wolff[1], Roland Gillen[1], Tamara Nagel[2], Jasmin Eisenkolb[2], Sabine Maier[1], Milan Kivala[3], Frank Hauke[2], Andreas Hirsch[2], and Janina Maultzsch[1] — [1]Chair of Experimental Physics, FAU Erlangen-Nürnberg, Erlangen — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg — [3]Organisch-Chemisches Institut, Centre for Advanced Materials, Universität Heidelberg

We present an innovative approach to achieve spatial variations in the degree of non-covalent functionalization of twisted bilayer graphene (tBLG). The tBLG with local twist angle variations between * 5° and 7° was non-covalently functionalized with 1,4,5,8,9,11- hexaazatriphenylenehexacarbonitrile (HATCN) molecules. We observe a correlation between the twist angle of tBLG and the degree of functionalization, determined through Raman spectroscopy. We propose that the adsorption of HATCN molecules follows the moiré pattern of twisted bilayer graphene, preferentially avoiding AA-stacked regions and primarily attaching to regions with local AB-stacking order, resulting in an overall ABA-stacking arrangement. This hypothesis, is further supported by density functional theory (DFT) calculations [1]. [1] Dierke et al., Angew. Chemie Int. Ed., accepted (2024), DOI: 10.1002/anie.202414593

DS 10: Transport Properties

Time: Thursday 11:30–12:30 Location: H14

DS 10.1 Thu 11:30 H14

A tunable room temperature nonlinear Hall effect in elemental bismuth thin films — •Pavlo Makushko[1], Sergey Kovalev[1], Yevhen Zabila[1], Igor Ilyakov[1], Alexey Ponomaryov[1], Atiqa Arshad[1], Gulloo Lal Prajapati[1], Thales V. A. G. de Oliveira[1], Jan-Christoph Deinert[1], Paul Chekhonin[1], Igor Veremchuk[1], Tobias Kosub[1], Yurii Skourski[1], Fabian Ganss[1], Denys Makarov[1], and Carmine Ortix[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V. — [2]Università di Salerno, Fisciano (SA), Italy

The nonlinear Hall effect with time-reversal symmetry is a second-order electronic transport phenomenon that induces frequency doubling and occurs in non-centrosymmetric crystals with Berry curvature dipole. This effect was typically reported in complex compounds characterized by Dirac or Weyl electrons at low temperatures. Here, we report a room temperature nonlinear Hall effect in polycrystalline thin films of the centrosymmetric elemental bismuth. The nonlinear transversal currents are induced by electrons at the (111) free surface, which possesses a Berry curvature triple. The nonlinear transverse voltage can be boosted by the geometric nonlinear Hall effect in arc-shaped bismuth stripes. The geometric curvature induced frequency doubling is extended to the second-harmonic generation in the terahertz spectral range. We also demonstrate efficient high-harmonic generation in polycrystalline bismuth films and bismuth-based heterostructures across a broad range of terahertz frequencies.

[1] P. Makushko et al., Nature Electronics 7, 207 (2024).

DS 10.2 Thu 11:45 H14

Electrochemical characterization of CeO_2/YSZ multilayer systems with well-defined interfaces — •Julius K. Dinter[1], Anja Henss[1,2], and Matthias T. Elm[1,2] — [1]ZfM, JLU Gießen — [2]Institute of Experimental Physics, JLU Gießen

Mixed ionic and electronic conductors (MIECs) are key components for a variety of electrochemical devices. Their functionality depends on their ability to store or transport both electrons and ions. However, most materials with high ionic conductivity exhibit poor electronic conductivity and vice versa. A common approach to overcome this challenge is the preparation of artificial mixed conductors by mechanically mixing a good electronic conductor with an ionic conductor. Consequently, these artificial MIECs are characterized by a high number of interfaces, which can significantly affect charge storage and charge transport in the composites. A detailed understanding of the impact of these interfaces on the electrochemical properties is essential for the design and improvement of electrochemical devices with enhanced functionality. We present the preparation and characterization of multilayer heterostructures of ceria (CeO_2) and yttria-stabilized zirconia (YSZ). The multilayers with constant thickness but varying number of interfaces were prepared by pulsed laser deposition to obtain thin film structures with well-defined interfaces. Structural characterization was performed using Raman microscopy and time-of-flight secondary ion mass spectrometry. The electrochemical properties were characterized by electrochemical impedance spectroscopy at different temperatures and under varying atmospheric conditions.

DS 10.3 Thu 12:00 H14

Magneto transport in bilayer graphene cavities — •Florian Schöppl[1], Michael Barth[1], Ming-Hao Liu[2], Klaus Richter[1], and Angelika Knothe[1] — [1]Institut für Theoretische Physik, 93053 Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan City 701, Taiwan

The remarkable sample quality of bilayer graphene in combination with the unprecedented electronic control of the band-structure makes bilayer-graphene an excellent platform for electron optics. While the purity of the system allows for ballistic transport on the micrometer scales [1,2], the trigonal warping of the band structure close to each

K points induces a valley dependent selection of momenta leading to unique transport and scattering properties [3,4]. Interested in the interplay of symmetry breaking induced by a variety of all-electronic gate confinements and the trigonal warping, we implement various quantum mechanical tight binding models as well as semiclassical simulations and deploy them to investigate magneto transport through bilayer graphene cavities.

[1]L. Seemann et al., Gate-tunable regular and chaotic electron dynamics in ballistic bilayer graphene cavities, Phys.Rev. B (2023) [2]L. Banszerus et al., Ballistic Transport Exceeding 28*m in CVD Grown Graphene, Nano Lett. 2016 [3]C. Gold et al., Coherent Jetting behind a gate-defined channel in bilayer graphene, Phys.Rev. Lett. (2021) [4]J.K. Schrepfer e t al. Dirac fermion optics and directed emession from single- and bilayer graphene cavities, Phys. Rev. B (2021)

DS 10.4 Thu 12:15 H14

Electrical transport across thin catalyst/defect-engineered titania corrosion protection layer interfaces for photoelectrochemical applications — •Julius Kühne[1,2], Tim Rieth[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technichal University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Producing value-added products via light-driven photoreduction represents a promising approach to sustainably address increasing CO2 emissions and meet the growing global energy demand. However, such solar fuels systems require passivating layers to chemically protect semiconductor light absorbers from harsh reaction environments. Despite great progress in the development of atomic layer deposited (ALD) protection layers, the factors governing efficient charge injection into the catalytic component remain not well understood. The nanoscale thickness of these ultrathin layers presents unique challenges, particularly for in-plane electrical measurements, complicating the reliable characterization of their transport properties compared to bulk materials. Here, the charge transport characteristics between various defect-engineered TiO2 protection layers grown with ALD and metal catalyst layers are investigated. By analyzing contact resistivity, carrier transport, and interface kinetics, this work seeks to deepen understanding of the interface between catalyst and protection layer.

DS 11: Thermoelectric and Phase Change Materials

Time: Thursday 15:00–16:00 Location: H3

DS 11.1 Thu 15:00 H3

Bond strength and force constants in RESbS — •Franziska Zahn[1], Christopher Benndorf[2], Hans H. Falk[1], Konrad Ritter[1], Sergiu Levcenko[1], Edmund Welter[3], Oliver Oeckler[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektron Synchrotron DESY, Hamburg, Germany

Our recent study on bond strength in different materials has shown that elemental Sb exhibits characterics of regular covalent and multicenter bonding based on the behavior of force constants with increasing interatomic distance. *RE*SbS are Sb-containing rare-earth (*RE*) pnictide chalcigenides that show special electronic and magnetic properties. They consist of different layeres, including Sb monolayers that alternate with *RE*-S double layers. To study the structural and vibrational properties of *RE*SbS with *RE* = La, Ce, Pr, and Nd in more detail, extended X-ray absorption fine structure spectroscopy (EXAFS) was performed at the Sb K-edge at ten different temperatures ranging from 20 to 295 K. The temperature dependence of the bond length variation σ^2 (mean square relative displacement) was evaluated using a correlated Einstein model, providing static disorder and force constants. The behavior of the force constants with incrasing interatomic distance is compared to other materials and to elemental Sb in particular. This contributes to the fundamental understanding of physical properties of *RE*SbS and their potential origin.

DS 11.2 Thu 15:15 H3

Enhancing mechanical flexibility and thermoelectric efficiency of amorphous TiNiSn — •Denis Music — Department of Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden

Thermoelectrics can convert heat to electricity without greenhouse gas emissions and hold significant potential as energy sources for wearable devices. Current research focuses on designing compounds that combine high conversion efficiency with mechanical flexibility. Half-Heusler phases, such as TiNiSn, demonstrate promising chemical stability and thermoelectric efficiency, but their inherent brittleness limits their application in flexible devices. To address this shortcoming, amorphous TiNiSn thin films were synthesized by sputtering on various substrates, such as Kapton, silk, and paper, to evaluate their bending response. These thin films show good adhesion to the substrates, as predicted by density functional theory, and do not delaminate under mechanical loading. Bending tests up to 154 degrees reveal minimal crack formation, indicating a high degree of flexibility. Consequently, amorphous TiNiSn is a promising candidate for flexible thermoelectric devices. To further enhance the thermoelectric efficiency of these devices, density functional theory and Boltzmann transport theory were employed to tune the electronic structure and identify suitable doping elements among 3d and 4d transition metals. Experiments were carried out to validate these predictions, yielding an order of magnitude increase in performance at room temperature.

DS 11.3 Thu 15:30 H3

Atomic arrangement in MBE grown chalcogenide thin films: structural investigation based on LEED-IV — •Maximilian Buchta[1], Christoph Ringkamp[1], Lucas Bothe[1], and Matthias Wuttig[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

If chalcogenides such as GeTe or Sb2Te3 are confined to reduced dimensions, for instance by reducing the film thickness, distortions in the atomic arrangement of the crystal emerge, which have been investigated by techniques such as X-ray diffraction (XRD). However, for the chalcogenides SnTe and SnSe, density functional theory (DFT) predicts pronounced distortions not only for thin films but also at the vicinity of the surface, which cannot be resolved by XRD. Further, as the distortions occur in both out-of-plane and in-plane directions, advanced structural characterization techniques are necessary to determine the atomic arrangement. In this work, Low Energy Electron Diffraction (LEED) Intensity vs. Electron Energy (LEED-IV) curves will be utilized to determine the surface atomic arrangement of tin-based chalcogenide thin films (SnTe and SnSe), grown by Molecular Beam Epitaxy (MBE), providing direct experimental evidence for structural predictions based on DFT.

DS 11.4 Thu 15:45 H3

Characterization of Nucleation and Growth Processes in the Phase Change Material GeTe upon Laser-Induced Switching — •Ramon Pfeiffer, Pascal Schröder, Elias Hildebrand, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

We have investigated how germanium telluride (GeTe) phase change material behaves during laser-induced switching at a wavelength of 658 nm. Starting with an amorphous GeTe matrix, which we have crystallized using laser pulses, GeTe has been reverted back to an amorphous state before recrystallizing it again. To analyze concomitant changes, we have examined individual crystal grains using electron backscatter diffraction (EBSD) and topographic changes by atomic force microscopy (AFM). Additionally, we have explored larger spot sizes during the second crystallization phase to assess the influence of a crystalline matrix on nucleation and growth dynamics within the material. These experiments revealed distinct nucleation and growth mechanisms that depend on the parameters used for crystallization.

DS 12: Gaede-Jubiläumssitzung

The Gaede Prize was founded 40 years ago by Dr Manfred Dunkel and is awarded annually for outstanding scientific work in basic research and application, for which the use of vacuum is relevant. To mark this anniversary, Selina Olthof (2019 prizewinner), Philip Willke (2022), Philip Hofmann (2011), and Andreas Waag (1998) from the illustrious list of prizewinners will give presentations in this session, covering a broad spectrum from the prize-relevant fields of thin films, surface science, semiconductor physics, and nanotechnology.

Time: Thursday 16:15–18:30 Location: H3

Invited Talk DS 12.1 Thu 16:15 H3

Probing the Electronic Structure of Halide Perovskites — •Selina Olthof — Department of Chemistry, University of Cologne — Chair of Material and Surface Analysis, University of Wuppertal

Halide perovskites are a novel class of thin film semiconductors that have revolutionized the field of photovoltaics, nowadays even surpassing in record efficiency the conventional silicon-based cells. Their remarkable defect tolerance, solution-based processability and tunable band gap make them highly promising for next-generation optoelectronic technologies.

This talk will provide a brief introduction to halide perovskites, highlighting the origins of their exceptional material properties. Next, I will introduce UV photoelectron spectroscopy (UPS) as well as reflection electron energy loss spectroscopy (REELS) as powerful tools to gain deeper insight into device relevant material properties. Specifically, I will discuss our investigations into the valence and conduction band density of states in tin and lead-based 3D perovskites. By combining photoelectron spectroscopy results with density functional theory, we identified the roles of atomic positions, bond hybridization, and lattice distortions in shaping the electronic properties.

Additionally, I will introduce our recent work on reduced-dimensionality perovskites (2D layers), which are gaining attention for their potential to optimize interfaces and enhance solar cell efficiencies. Here, I will present a systematic study using alkyl-based organic cations with varying chain length, which we used to track effects of interlayer spacing on the electronic and optical properties.

Invited Talk DS 12.2 Thu 16:45 H3

Quantum Science with Single Atoms and Molecules on Surfaces — •Philip Willke — Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

The quantum nature of a physical system often emerges from its fundamental building blocks and demands a deep understanding to leverage its benefits for future quantum devices. In this talk, I introduce the combination of electron spin resonance (ESR) and scanning tunneling microscopy (STM) as a new platform for coherent control of spins on surfaces (1). This technique enables for instance the addressing of individual atoms on surfaces with exceptional energy resolution. It allowed for high-resolution magnetic sensing, for instance by resolving their hyperfine interaction between the electron and nuclear spins. Recently, we have extended this technique to achieve spin resonance on individual molecules (2), which is particularly exciting as it extends ESR-STM into the realm of molecular quantum technologies: Promising new avenues involve organizing spins through molecular self-assembly into larger structures, alongside the application of on-surface chemistry techniques. As an example, we demonstrate how constructing new complexes through tip-assisted on-surface assembly can lead to spin systems with improved dynamic spin properties (3), that can be coherently controlled. (1) Chen, Y. et al., Advanced Materials, 35 (27), 2107534 2023. (2) Zhang, X. et al. Nat. Chem., 14, 59-65 2022. (3) Huang, W. et al. arXiv.2410.18563 2024.

session break

Invited Talk DS 12.3 Thu 17:30 H3

Gallium Nitride Technology - the second pillar of microelectronics — •Andreas Waag — Nitride Technology Center NTC, TU Braunschweig

The highly efficient radiative recombination makes GaN ideally suited for microLEDs with dimensions as small as 1 μm and even below. Besides display applications, their capability to produce optical patterns with high resolution, which can be modulated at extremely high frequencies, makes them suitable for numerous other applications.

Besides chip-based microscopy and highly efficient sensing, we explore these exciting properties for a new highly significant application: utilizing microLEDs in optical processing units for artificial intelligence workloads.

The talk will focus on technological challenges of chip processing and hybrid integration with silicon CMOS microelectronics. For all these applications, nitride technology and the exciting properties of GaN semiconductor devices are a key.

Invited Talk DS 12.4 Thu 18:00 H3

Ultrafast X-ray photoelectron spectroscopy and photoelectron diffraction — •Philip Hofmann — Department of Physics and Astronomy, Aarhus University, Denmark

X-ray photoelectron spectroscopy (XPS) is an experimental tool capable of accurately determining the core level binding energies of atoms. This energy is not only element-specific but also provides detailed information on the atoms' oxidation state and chemical environment, making XPS an essential tool for studying catalytic processes. XPS line shapes have also attracted considerable interest, leading to the development of many-body theories to study the solid's electronic and vibrational properties. Finally, the core level photoemission intensity can be interpreted as a diffraction pattern that gives access to the emitting atom's local geometrical environment in an experimental approach called X-ray photoelectron diffraction (XPD).

The increasing availability of ultrafast X-ray sources at free electron lasers now opens the opportunity to take XPS and XPD into the ultrafast time domain and this talks will give two recent examples. For graphene, it is shown that a study of the time-dependent XPS line shape can reveal detailed insight into the excitation of the system, directly giving access to parameters such as the electronic temperature. A demonstration of XPD is given in which the motion of surface atoms of the topological insulator Bi_2Se_3 is tracked after the excitation of a coherent optical phonon.

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 selectivity. 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 [$Bi_{38}O_{45}$(Boc-L-Met-O)$_{24}$] or [$Bi_{38}O_{45}$(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

[3] A. Coughlin et al., ACS Materials Letters, 5 (2023) 1945-1953.

DS 13.24 Thu 18:00 P1

Investigating interfacial mechanisms and switching behavior in GST-124/Sb$_2$Te$_3$ 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$_2$Te$_4$ (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$_2$Te$_3$ 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 $(FeCrNi)_xTe$ 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.

[1] Z. Zhang et al., Chemical Engineering Journal 2024, 498, 155736.
[2] A. Tschesche et al., R.S., doi.org/10.21203/rs.3.rs-4861088/v1.
[3] N. Oueldna, Materials Horizons 2024, 11(10), 2323-2354.

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.

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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 Oberflächenforschung, Technische Universität Darmstadt

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.

References

[1] P. T. Ahmadi, et al. Journal of Vacuum Science & Technology A 42, 063402 (2024).

[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 ($T>335$K), 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] —

[1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 3, 07743 Jena, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Lessingstraße 12-14, D-07743 Jena, Germany — [3]Helmholtz Institute Jena, Fröbelstieg 3, D-07743 Jena, Germany

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 $(\mathrm{GeTe})_x(\mathrm{SnTe})_{1-x}$ 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 $(\mathrm{GeTe})_x(\mathrm{SnTe})_{1-x}$ 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.

DS 14: Members' Assembly

Time: Thursday 18:30–20:00 Location: H3

All members of the Thin Films Division are invited to participate.

DS 15: Organic Thin Films, Organic-Inorganic Interfaces

Time: Friday 9:30–11:45 Location: H3

Invited Talk DS 15.1 Fri 9:30 H3

Structure formation and growth at the metal-organic interface — •Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University Linz, Austria

The evolution of the structural, electronic and optical properties of organic thin films strongly depend on the ordering, aggregation and orientation of the molecules within the very first or a few deposited monolayers. The chosen substrate and its intentional modification (e.g. by pre-adsorption of inorganic or organic species) may thus have a strong influence on the structural, electronic and optical properties of the growing organic thin film. Using complementary experimental methods, namely, surface optical spectroscopy (RDS, DRS), diffraction (LEED) and microscopy (STM, PEEM), supported by empirical models and ab-initio calculations we aim to identify (and eventually quantify) the underlying driving forces. We will present examples on the 2D condensation of organic molecules on metal surfaces, the structural and orientational ordering in 2D (and quasi 1D) monolayer phases and its influence on the further growth of the organic thin film. Finally, we will illustrate the effects of modification / templating of the substrate on the structure and properties of the organic layers.

DS 15.2 Fri 10:00 H3

Thin film heterostructures based on Co/Ni synthetic antiferromagnets on polymer tapes: towards a sustainable flexible spintronics — •Mariam Hassan[1], Sara Laureti[2], Christian Rinaldi[3], Federico Fagiani[3], Gianni Barucca[4], Manfred Albrecht[5], and Gaspare Varvaro[2] — [1]Institute of Physics, TU Chemnitz, Germany — [2]CNR-ISM, nM2-Lab, Italy — [3]Department of Physics, Politecnico di Milano, Italy — [4]Università Politecnica delle Marche, Dipartimento SIMAU, Italy — [5]Institute of Physics, University of Augsburg, Germany

The PGMs-free Co/Ni-system offers several advantages for spin-based devices such as low damping and high spin polarization, and they contribute to a more sustainable future. Moreover, these films could be good substrates for the investigation of the chiral-induced spin selectivity "CISS" effect. In this work, flexible synthetic-antiferromagnets with perpendicular-magnetic-anisotropy (PMA-SAFs) and GMR-spin-valves (SVs) containing a SAF-reference electrode and a Co/Ni-free layer were deposited on flexible polyethylene naphthalate tapes with different combinations of buffer and capping layers (Pt, Pd, Cu/Ta). High-quality SAFs with a fully compensated antiferromagnetic region and SVs with a sizeable GMR ratio were obtained. The best performances are achieved with PGMs used as buffer layer and Cu as capping layer[1]. The results indicate that complex Co/Ni-based heterostructures with reduced content of PGMs deposited on flexible tapes allow for the development of novel shapeable and sustainable spintronic devices. [1]ACS Appl. Mater. Interfaces. 14 (2022) 51496-51509.

DS 15.3 Fri 10:15 H3

highly crystalline, cleavable, and transferable semiconducting 2D imine COF film — •diksha srivastava[1], vipin mishra[2], showkat h. mir[3], jyotirban dey[1], jayant k. singh[1], manabendra chandra[1], and thiruvancheril g. gopakumar[1] — [1]Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]KU Leuven, Celestijnenlaan 200F, Leuven B-3001, Belgium — [3]University of Kashmir, Hazratbal, Srinagar 190006, Jammu and Kashmir, India

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are emerging crystalline organic polymers with potential applications in thin-film electronics, sensing, and catalysis, driven by their stability, tunable electronic properties, and versatile functionality. We present a scalable method for synthesizing 2D imine-COF films on dielectric glass substrates via a Schiff base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA) over 15 hours. This yields highly crystalline 2D networks with film thicknesses ranging from 100 nm to a few monolayers and lateral dimensions up to 2 cm. Sonication exfoliation is employed for producing free-standing films. Structural characterization via SEM, TEM, and AFM confirms highly crystalline 2D structures. XPS analysis validates the chemical composition, while optical measurements indicate a semi-conducting band gap. DFT calculations show a semiconductor-like band structure with strong band dispersion near the conduction and valence band edges, signifying efficient charge transport and potential for future electronic applications.

session break

DS 15.4 Fri 10:45 H3

Excited state dynamics in thin films of planar and twisted azaperopyrene derivatives — •Jakob Steidel[1], Robert Eichelmann[2], Jakob Sawatzki[1], Lutz Gade[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, Germany

Azaperopyrene derivatives are a class of organic semiconductors with a high potential for applications in optoelectronic devices. The molecular π-system of planar octaazaperopyrenedioxide (OAPPDO-H) is substituted with chlorine yielding OAPPDO-Cl, a molecule with a twisted structure.

In this contribution we utilised transient absorption spectroscopy to elucidate excited state dynamics of OAPPDO derivatives with planar and twisted molecular π-systems in thin films. On a short time scale of several hundred femtoseconds we observed fast population of excited states and fluorescence in both materials. The lifetimes of these processes show a similar dependency on the intensity of the excitation pulse. On a long time scale of several nanoseconds striking differences were observed. While the lifetimes of the excited state in OAPPDO-Cl increased and saturated with increasing excitation intensity, the lifetimes in OAPPDO-H showed a maximum at a medium excitation intensity of 400 nJ per pulse. We assign this behaviour to the opening of an additional decay pathway due to triplet-triplet-annihilation that requires cofacial arrangement of two molecules. Only planar OAPPDO-H can arrange in such a way, while the increased steric hindrance in OAPPDO-Cl suppresses this intermolecular interaction.

DS 15.5 Fri 11:00 H3

Thermally Tuning the Optical Properties of Discrete NDI-T2 Oligomer Thin Films — •Alexander Ehm[1], Fabian Eller[2], Meike Kuhn[2], Rukiya Matsidik[1], Michael Sommer[1], Eva M. Herzig[2], and Dietrich R. T. Zahn[1] — [1]Faculty of Natural Sciences, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, D-95447 Bayreuth, Germany

In the pursuit of developing and optimizing n-type organic semiconductors for the use in organic electronics, materials derived from naphthalene diimide (NDI) and bithiophene (T2), such as P(NDI2OD-T2), are highly interesting [1]. Changing the average molecular orientation via thermal annealing, and thereby their opto-electronic properties, allows finetuning for specific applications [2].

Recently, we showed that the optical anisotropy of the discrete oligomers NDI-(T2-NDI)2 and T2-(NDI-T2)2 can be influenced by thermal annealing [3]. Here, we extend this study and reveal that the photoluminescence and optical anisotropy, as found by variable-angle spectroscopic ellipsometry of T2-(NDI-T2)2 can be continuously tuned by the choice of the annealing temperature. The correlation with molecular alignment is investigated using grazing-incidence wide-angle X-ray scattering.

[1] Chen et al. J. Am. Chem. Soc. 2009, 131, 8
[2] Vu et al. ACS Macro Lett. 2023, 12, 140
[3] Ehm et al. Phys. Status Solidi B Basic Res. 2024, 2400202

DS 15.6 Fri 11:15 H3

Highly-Robust Double Neuromorphic Device Based on Perovskite/Molybdenum Oxide-Sulfide Compound Heterojunction — •Gion Kalemai[1,2], Michael-Alexandros Kourtis[3], Anastasia Soultati[1], Apostolos Verykios[1], Dimitris Davazoglou[1], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology (INN) National Center for Scientific Research Demokritos, Agia Paraskevi, Athens, Greece — [2]Department of Physics, University of Patras, Patra Rio, Greece — [3]Institute of Informatics & Telecommunications, National Center for Scientific Research Demokritos, Agia Paraskevi, Athens, Greece

This study addresses the fundamental perovskite memristor limitations by integrating a robust molybdenum oxide-sulfide (MoO3-MoS2) mixed layer beneath a RbCsMAFA quadruple cation perovskite, precisely engineered through sulfurization of sub-stoichiometric MoO3-x. The resulting neuromorphic device exhibits impressive RS, with an ON-OFF ratio of 100, high retention & endurance, and a 0.5sec switching speed. Analysis confirm the successful control in the MoO3-MoS2 structure, which introduces trap states within the bandgap, facilitating SCLC and enabling robust memory function.

The composite, demonstrates enhanced synaptic emulation capabilities, such as PPF-PPD, and STP-LTP, replicating key synaptic functions for neuromorphic computing. Notably, this device offers excellent stability under 85°C, an enhanced ON-OFF ratio under illumination. Thus, the potential of sub-stoichiometrically engineered architectures is underlined.

DS 15.7 Fri 11:30 H3

Spatially resolved work-function manipulation of azobenzene-functionalized self-assembled monolayers by optical stimulation — Jan Böhnke[1], Beatrice Andres[1], Larissa Boie[1,2], Angela Richter[1], Cornelius Gahl[1], Martin Weinelt[1], and •Wibke Bronsch[1,3] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen, Switzerland — [3]Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14-km 163.5 in AREA Science Park, 34149 Basovizza, Trieste, Italy

Strongly differing static dipole moments of the trans and cis isomers of photochromic azobenzene allow for optical work-function switching of azobenzene-functionalized self-assembled monolayers (SAMs) [1,2]. We apply these properties in a fundamental experiment to manipulate the area size of the switched SAM [3]. In our experiments we spatially resolve the transient isomerization profile of the SAM after UV illumination by means of photoemission electron microscopy imaging. We demonstrate the capability of spatial tuning of the SAM's work function and discuss the role of the laser spot profile in generating sharp edges or gradual changes of the work function across the sample.

[1] Bronsch et al., Appl. Phys. Lett. 111, 081601 (2017).
[2] Bronsch et al., J. Phys.: Condens. Matter 29, 484002 (2017).
[3] Böhnke et al., Appl. Phys. Lett. 124, 191601 (2024).