Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls REC/B214 and REC/C213; Poster P2)

Invited Talks

DS 6.1	Tue	9:30–10:00	REC/C213	**Soft X-ray Microscopy of Ferroic Thin Films** — •Tim A. Butcher, Simone Finizio, Michael Schneider, Jörg Raabe, Stefan Eisebitt, Bastian Pfau
DS 6.6	Tue	11:15–11:45	REC/C213	**Charge transfer at interfaces of free-standing oxide membranes and heterostructures** — Kapil Nayak, Lee-Kang Huang, Anton Kaus, Marcus Wohlgemuth, Alexandros Sarantopoulos, Christoph Baeumer, Regina Dittmann, •Felix Gunkel
DS 13.1	Wed	15:00–15:30	REC/B214	**Tailored thermal treatments for multi-layer, multi-material polymer devices** — •Katherina Haase, Shaoling Bai, Mike Hambsch, Vojtech Millek, Stefan C. B. Mannsfeld
DS 18.8	Thu	17:00–17:30	REC/C213	**Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces** — •Frank Ortmann

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium Tipping Points in Social and Climate Systems (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

DS 1.1–1.3	Mon	9:30–10:15	REC/C213	**Organic Thin Films**
DS 2.1–2.7	Mon	15:00–18:15	HSZ/0003	**Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)**
DS 3.1–3.4	Mon	15:00–16:00	REC/C213	**Thin Film Properties I: Methods**
DS 4.1–4.6	Mon	16:30–18:15	REC/C213	**Thin Film Properties II**
DS 5.1–5.4	Tue	9:30–10:45	HSZ/0105	**Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)**
DS 6.1–6.6	Tue	9:30–11:45	REC/C213	**Thin Oxides and Oxide Layers**
DS 7.1–7.5	Tue	10:00–11:30	REC/B214	**Thermoelectric and Phase Change Materials**
DS 8.1–8.5	Tue	14:00–15:30	REC/B214	**Transport Properties**
DS 9.1–9.5	Tue	14:00–15:15	REC/C213	**Thin Film Properties III: Oxides**
DS 10.1–10.7	Wed	9:30–12:45	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)**
DS 11.1–11.8	Wed	9:30–11:45	REC/B214	**Layer Deposition**
DS 12.1–12.9	Wed	9:30–12:00	REC/C213	**2D Materials I**
DS 13.1–13.4	Wed	15:00–16:15	REC/B214	**Layer Properties**
DS 14.1–14.9	Wed	15:00–17:30	REC/C213	**2D Materials II (joint session DS/HL)**
DS 15.1–15.11	Thu	9:30–12:30	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)**
DS 16.1–16.10	Thu	9:30–12:30	REC/C213	**Thin Film Application**
DS 17.1–17.9	Thu	15:00–18:45	HSZ/0003	**Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)**
DS 18.1–18.8	Thu	15:00–17:30	REC/C213	**Spins in Molecular Systems**
DS 19	Thu	17:45–18:30	REC/C213	**Members' Assembly**
DS 20.1–20.52	Thu	18:30–20:30	P2	**Poster**
DS 21.1–21.10	Fri	9:30–12:30	REC/C213	**Optical Analysis of Thin Films**

Members' Assembly of the Thin Films Division

Thursday 17:45–18:30 REC/C213

DS 1: Organic Thin Films

Time: Monday 9:30–10:15 Location: REC/C213

DS 1.1 Mon 9:30 REC/C213

Thin film growth on weak surfaces: influence of substrate inhomogeneities — •Eric Karajic[1], Martin Oettel[1], Edwin Mozo[2], and Fabio Reis[2] — [1]University of Tübingen, Institute of Applied Physics — [2]Universidade Federal Fluminense, Instituto de Fisica

The initial island density in the growth of thin films on perfectly smooth surfaces is set by an interplay between flux, diffusion and the stability of small clusters [1]. However, real surfaces have inhomogeneities which may trap freely diffusion adsorbates and act as initial nucleation sites. Using kinetic Monte-Carlo (KMC) simulations, we investigate the influence of trapping strength and density of inhomgeneities on the initial growth behavior. We discuss the consequences for basic growth modes on weakly interacting surfaces [2]. For layer-by-layer growth, island densities may vary grossly between first and second layer, but for island growth the possible return to smooth growth at intermediate layer thicknesses is not affected. [1] T. Michely and J. Krug, Islands, Mounds, and Atoms, (Springer, 2003) [2] E. Empting et al., Phys. Rev. E 103, 023302 (2021)

DS 1.2 Mon 9:45 REC/C213

Organic self-assembled monolayers as barrier material in Josephson junctions — •Moritz Singer[1], Harsh Gupta[1], Rui Pereira[2], Benedikt Schoof[1], and Marc Tornow[1,2] — [1]TU Munich, Garching, Germany — [2]Fraunhofer EMFT, Munich, Germany

Superconducting qubits employ Josephson junctions (JJs) to provide the non-linearity needed to address a unique two-state system. The JJs consist of two superconducting electrodes which are separated by a nanometer-thin layer acting as tunnel barrier and is mostly fabricated from oxides. The thickness of the oxide is highly sensitive to process variations, and it hosts many two-level systems (TLS) which give rise to dielectric losses, thereby limiting the qubit coherence times. In this study, we report on JJs comprising an organic self-assembled monolayer (SAM) as the insulating barrier material. Our JJs consist of Ta electrodes on a Nb seed layer, separated by a SAM of octadecene (C18H36) molecules that are grown on the thin native TaOx layer of the bottom electrode. We fabricated JJs with three different electrode sizes in the μm - range and measured critical currents Ic between 3.7 μA and 30.6 μA at 100 mK, in good quantitative agreement with the expected values according to the Ambegaokar-Baratoff relation. We further analyzed the data using the Simmons tunneling model, adapted to account for the two-layer TaOx/SAM barrier. We obtain barrier heights ranging from 0.43-0.57 eV for the SAM-JJs, which is significantly higher than for JJs fabricated with a Ta-oxide barrier only (barrier height 0.25 eV). This shows that the properties of JJs can be modified and tuned by introducing a SAM as barrier material.

DS 1.3 Mon 10:00 REC/C213

Prediction of room-temperature two-dimensional pi-electron half-metallic ferrimagnet — •Jan Phillips[1], João C. G. Henriques[1,2], Antonio T. Costa[1,3], and Joaquín Fernández-Rossier[1,4] — [1]International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — [2]Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain — [3]Universidade do Minho, R. da Universidade, 4710-057 Braga, Portugal — [4]On permanent leave from Departamento de Física Aplicada, Universidad de Alicante, 03690 San Vicente del Raspeig, Spain

We propose a strategy to obtain conducting organic materials with fully spin-polarized Fermi surface, lying at a singular flat band, with antiferromagnetically coupled magnetic moments that reside in pi-orbitals of nanographenes. We consider a honeycomb crystal whose unit cell combines two molecules with S=1/2: an Aza-3-Triangulene, a molecule with orbital degeneracy, and a a 2-Triangulene. The analyzed system is half-metallic with a ferrimagnetic order, presenting a zero net total magnetic moment per unit cell. We combine density functional theory calculations with a Hubbard model Hamiltonian to compute the magnetic interactions, the bands, and the collective spin excitations. We obtain very large intermolecular exchange couplings, in the range of 50 meV, which ensures room temperature stability. This crystal being a half-metal with fully compensated magnetic moments combines two characteristics that would make it ideal for spintronics applications.

DS 2: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g, via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15 Location: HSZ/0003

Topical Talk DS 2.1 Mon 15:00 HSZ/0003

Charge confinement in twisted bilayer graphene — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Twisted bilayer graphene (tBLG) near the magic angle is a unique platform where the combination of topology and strong correlations gives rise to exotic electronic phases. These phases are gate-tunable and related to the presence of flat electronic bands, isolated by single-particle band gaps. This enables charge confinement and allows to explore the interplay of confinement, electron interactions, band renormalisation and the moiré superlattice, potentially revealing key paradigms of strong correlations. In this talk we will present two experiments where we study charge confinement in tBLG. First, we report on the observation of negative electronic compressibility in tBLG for Fermi energies close to insulating states. To observe this negative compressibility, we take advantage of naturally occurring twist-angle domains that emerge during the fabrication of the samples, leading to the formation of charge islands. Second, we present gate-defined single-electron transistors (SETs) in near-magic-angle tBLG with well-tunable Coulomb blockade resonances. These SETs allow to study

magnetic field-induced quantum oscillations in the density of states of the source-drain reservoirs, providing insight into gate-tunable Fermi surfaces of tBLG and open the door to quantum dots and Josephson junction arrays in tBLG.

Topical Talk DS 2.2 Mon 15:30 HSZ/0003

Tuning Coulomb interactions and Hubbard bands in 1T-TaS_2 — •Anna Galler — Institute of Theoretical and Computational Physics, TU Graz, Austria — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Monolayer 1T-TaS_2 hosts a star-of-David charge-density wave (CDW) that stabilizes a low-temperature Mott-insulating state. Recent time-resolved spectroscopies indicate a coupling between the CDW amplitude mode and the electronic correlation strength, yet the role of the screened Coulomb interaction remains unclear. Using the constrained random-phase approximation, we show that the CDW amplitude modifies the bare and screened on-site interactions, leading to sizable variations in the effective Hubbard U. Our combined density-functional and dynamical mean-field theory calculations reveal that the Hubbard bands shift in concert with the CDW amplitude, and that a reduced distortion drives a transition from a Mott insulator to a correlated metal. These results demonstrate a direct link between lattice distortions and Coulomb interactions in transition-metal dichalcogenides, providing a microscopic mechanism for light-induced control of correlated phases in two-dimensional quantum materials.

Topical Talk DS 2.3 Mon 16:00 HSZ/0003

Optical signatures of interlayer electron coherence in a bilayer semiconductor — •Nadine Leisgang[1,2], Xiaoling Liu[2], Pavel Dolgirev[2], Philip Kim[2], and Mikhail Lukin[2] — [1]Phillips-Universität Marburg, Germany — [2]Harvard University, United States

Emergent strongly correlated electronic phenomena in atomically thin transition-metal dichalcogenides represent an exciting frontier in condensed matter physics, with examples ranging from bilayer superconductivity and electronic Wigner crystals to the ongoing search for exciton condensation. Here, we take a step towards the latter by reporting experimental signatures of unconventional coupling of interlayer excitons consistent with coherence between interlayer electrons in a transition-metal dichalcogenide bilayer. We investigate naturally-grown MoS_2 homobilayers integrated in a dual-gate device structure allowing independent control of the electron density and out-of-plane electric field. When the bilayer is electron-doped under conditions where tunnelling between layers is negligible, we observe that two interlayer excitons - which normally should not interact - hybridize in a way distinct from both conventional level crossing and anti-crossing. We show that these observations can be explained by quasi-static random coupling between the excitons, which increases with electron density and decreases with temperature. We argue that this phenomenon is indicative of a spatially fluctuating order parameter in the form of interlayer electron coherence - a theoretically predicted many-body state that has yet to be unambiguously established experimentally outside the quantum Hall regime.

15 min. break

Topical Talk DS 2.4 Mon 16:45 HSZ/0003

Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures — •Ammon Fischer — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — Center for Computational Quantum Physics, Flatiron Institute, New York, NY 10010, USA

Moiré materials - twisted stacks of two-dimensional materials - bridge between two influential paradigms of condensed matter research: nontrivial quantum geometry and strong electron-electron interactions. In this talk, I will outline how the construction of faithful low-energy models and their successive treatment by state-of-the-art many-body techniques allows to resolve electronic order in moiré and non-moiré heterostructures from first principles. In twisted bilayers of WSe_2, functional renormalization group techniques allow to unravel the angle evolution of antiferromagnetic order and superconductivity in the crossover regime from weak-to-moderate interactions. In rhombohedral multilayer graphenes, the low-energy theory is naturally described in terms of supercell Wannier functions that span the effective $U(4) \times U(4)$ subspace of the spin, valley and layer degrees of freedom. Electronic correlations give rise to various iso-spin ordered regimes, superconductivity and charge density wave order at low electronic densities bridging to the physics of their twisted counterparts.

Topical Talk DS 2.5 Mon 17:15 HSZ/0003

Mesoscale Atomic Engineering in a Crystal Lattice — •Julian Klein — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

Controlling the arrangement of individual atoms with lasers, ion traps, and scanning probe techniques has enabled quantum simulation and computing platforms that transcend naturally occurring configurations of matter. Yet achieving comparable atomic control within a solid and at scale remains a foundational challenge, one that could revolutionize the design of artificial matter. Here, I demonstrate atomic engineering of artificial matter inside a scanning transmission electron microscope. By developing strategies to position and move the electron beam with few-picometer accuracy, deterministic control over atomic motion in both space and time is achieved. Full automation of the microscope enables the creation of three-dimensional defect superlattices in many-nanometer thick CrSBr with user-defined lattice spacing and symmetry, spanning tens of thousands of engineered sites over fields of view exceeding one hundred nanometers, all generated in under an hour. Our results establish atomic engineering in the electron microscope as a practical reality, opening unprecedented opportunities to create quantum defects and quantum phases with tunable charge and spin interactions, and to control host-lattice excitations by arranging atoms in patterns that are commensurate or incommensurate with the underlying crystal over mesoscopic, and potentially micro- or macroscopic, length scales.

DS 2.6 Mon 17:45 HSZ/0003

Interlayer electrodynamics of CDWs in van der Waals materials and heterostructures — Achyut Tiwari, Renjith Mathew Roy, Maxim Wenzel, Christian Prange, Bruno Gompf, and •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Layered transition metal dichalcogenides such as 1T-TaS_2, 2H-TaS_2 and their natural heterostructure $4H_b$-TaS_2 provide a platform for studying interlayer coupling, orbital hybridization, and charge transfer that determine collective electronic phenomena, such as unconventional superconductivity and strong electronic correlations. Temperature-dependent infrared measurements of the in-plane and out-of-plane optical response of 1T-TaS_2 across its CDW-driven metal-insulator transition are combined with DFT calculations. We find that a quasi-1D instability that induces interlayer dimerization is responsible for the MI-transition. Furthermore, spectroscopic ellipsometry combined with an anisotropic Bruggeman effective medium approximation reveals that metallic domains evolve in a strongly anisotropic way and often extend along the out-of-plane direction as the transition proceeds.

When 1T-TaS_2 is stacked between 1H-TaS_2, forming a natural heterostructure of $4H_b$-TaS_2, charge transfer occurs between the layers, that can be tuned with temperature, and which is related to the CDW in 1T-TaS_2 layer. We conclude that the phase transition in 1T-TaS_2 is inherently three dimensional, despite its layered structure, and that interlayer coupling is essential for its electronic structure and phase behavior both individually and in heterostructures.

DS 2.7 Mon 18:00 HSZ/0003

Enhancing Plasmonic Superconductivity in Layered Materials via Dynamical Coulomb Engineering — •Yann in 't Veld[1], Mikhail I. Katsnelson[2,3], Andrew J. Millis[4,5], and Malte Rösner[2,6] — [1]I. Institute of Theoretical Physics, Universität Hamburg, Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [3]Constructor Knowledge Institute, Constructor University, Bremen, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, United States of America — [5]Department of Physics, Columbia University, New York, United States of America — [6]Faculty of Physics, Bielefeld University, Bielefeld, Germany

Conventional Coulomb engineering, through controlled manipulation of the environment, offers an effective route to tune the correlation properties of atomically thin van der Waals materials via static screening. Here we present tunable *dynamical* screening as a method for precisely tailoring bosonic modes to optimize many-body properties. We show that "bosonic engineering" of plasmon modes can be used to enhance plasmon-induced superconducting critical temperatures of layered superconductors in metallic environments by up to an order of magnitude, due to the formation of interlayer hybridized plasmon modes with enhanced superconducting pairing strength. We determine

optimal properties of the screening environment to maximize critical temperatures. We show how bosonic engineering can aid the search for experimental verification of plasmon mediated superconductivity.

DS 3: Thin Film Properties I: Methods

Time: Monday 15:00–16:00 Location: REC/C213

DS 3.1 Mon 15:00 REC/C213

Update on the IBA activities in Bonn — •Henry Schumacher, Dennis Sauerland, and Sebastian Neubert — Helmholtz-Institut für Strahlen und Kernphysik, Universität Bonn

The *Bonn Isochronous Cyclotron* can accelerate protons, deuterons and light ions with nominal energies of 7 to 14 MeV/nucleon. At one of the five beam lines, a new experimental site for material analysis is in development.
This new experiment will house a small number of surface barrier detector for RBS (backwards direction) and beam characterization (off-axis, foward direction) as well as a silicon drift detector for PIXE measurements and utilize a low energy alpha particle beam.
In this talk, a general overview over the setup and progress, preliminary detector tests, count rate estimations and preparatory measurements will be presented.

DS 3.2 Mon 15:15 REC/C213

The TXPES Beamline at SESAME: A New Facility for Advanced Soft X-ray Photoelectron Spectroscopy — •Zeynep Reyhan Ozturk — TARLA, Ankara, Turkey — SESAME, Balqa, Jordan

The TXPES (Turkish X-ray Photoelectron Spectroscopy) beamline at SESAME is a newly installed soft X-ray facility dedicated to high-resolution XPS, UPS, and ARPES for advanced surface and interface analysis. With a broad tunable photon-energy range, TXPES enables detailed investigation of electronic structure, chemical composition, band dispersion, and oxidation states in a wide variety of materials.

The end station features a multi-chamber UHV system including a preparation chamber, an analysis chamber, and a high-pressure cell for in situ and near-ambient pressure studies. The analysis chamber houses a hemispherical electron energy analyzer capable of XPS/UPS/ARPES, along with an ion gun, LEED, and LEIS, enabling comprehensive structural and chemical characterization at different depth sensitivities. TXPES combines tunable soft X-rays, high-resolution electron spectroscopy, and controlled environments to study surface oxidation, adsorption, catalysis, thin-film interfaces, and electronic band alignment with exceptional sensitivity. The integration of a high-pressure cell expands these investigations to realistic gas conditions, bridging the gap between model systems and real-world applications. The beamline represents a major collaborative effort between Turkish institutions and SESAME and is progressing toward full operation and user access in the near future.

DS 3.3 Mon 15:30 REC/C213

Bringing Synchrotron-Level HAXPES to the Lab: DeepCore-X for Buried Interface Characterization — •Martin Schmid[1], Elin Cartwright[2], Eleni Anargirou[1], Marcus Lundwall[2], and Susanna Eriksson[2] — [1]Scienta Omicron GmbH, Limburger Str. 75, 65232 Taunusstein — [2]Scienta Omicron AB, Danmarksgatan 22, 75323 Uppsala

Buried interfaces in multilayer semiconductor devices, such as MOSFETs, solar cells, and memory architectures, critically impact performance and reliability. Hard X-ray Photoelectron Spectroscopy (HAXPES), with greater information depth than conventional XPS, enables nondestructive analysis of buried layers. We introduce DeepCore-X, a next-generation lab instrument combining soft and hard XPS in one system, delivering synchrotron-like performance. Powered by a Ga Kα MetalJet source (9.25 keV), it offers 1000 W continuous operation and a hundred-fold intensity advantage over other lab HAXPES sources. The system supports high-throughput measurements across complex stacks. Automated sample handling, multi-point acquisition, and operando bias capabilities make it ideal for evaluating band bending, trap states, and chemical shifts. We will present recent results and application examples, including non-destructive depth profiling, to demonstrate how DeepCore-X bridges the gap between surface analysis and full device stack characterization without requiring synchrotron access.

DS 3.4 Mon 15:45 REC/C213

Simulation-Guided GIXPS: How to Maximize Signal and Depth Sensitivity in Photoelectron Emission Experiments — •O. Rehm[1], E. Kusari[1], D. Capalbo[1], A. Gloskovskii[2], C. Schlueter[2], L. Baumgarten[3], and M. Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]DESY, 22607 Hamburg — [3]FZ Jülich GmbH, PGI-6, 52425 Jülich

(Hard) X-ray Photoelectron Spectroscopy ((HA)XPS) is a powerful technique for probing the chemical and electronic structure of thin films, interfaces, and multilayers, but access to synchrotron radiation is typically highly limited. To address this constraint, we present a simulation-guided approach that optimizes (HA)XPS experiments through grazing-incidence (GI) geometries. At GI angles (0.3°-2°) refraction and total reflection of X-rays generate pronounced angle-dependent interference effects that shift the weighted contribution maximum of photoelectrons to well-defined depths within the sample. Our approach - GIXPS - predicts these conditions in advance, enabling targeted enhancement of surface, interface, or bulk sensitivity. It boosts photoemission intensity by up to two orders of magnitude at characteristic GI angles, enabling faster data acquisition and better depth resolution while preserving the element-specificity of (HA)XPS. This methodology provides a practical route to more efficient, depth-selective experiments and is a powerful tool for designing and carrying out optimized interface- and bulk-sensitive (HA)XPS measurements - thus enabling the more efficient use of limited synchrotron beamtime. O. Rehm *et al.*

DS 4: Thin Film Properties II

Time: Monday 16:30–18:15 Location: REC/C213

DS 4.1 Mon 16:30 REC/C213

Epitaxial Growth and Structural Characterization of Non-centrosymmetric B20-PtAl Thin Films — •Ayusa Aparupa Biswal[1], Darius Pohl[2], Bernd Rellinghaus[2], Edouard Lesne[1], and Claudia Felser[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — [2]Dresden Center for Nanoanalysis (DCN), cfaed, TU Dresden, Dresden, Germany

Topological chiral semimetals with the non-centrosymmetric cubic B20 structure (space group P213) are distinguished by chirality in their crystal, magnetic, and electronic structures [1]. B20 compounds do not possess inversion or mirror symmetry but preserve rotational symmetries. Non-magnetic B20 compounds, such as CoSi, RhSi, PdGa, and PtAl, host multifold fermions originating from topological band crossings. These lead to large Chern numbers and produce Fermi arcs, alike those found in Weyl semimetals [2,3]. We report on the heteroepitaxial growth of crystalline PtAl thin-films with a non-centrosymmetric cubic B20 structure. We employ magnetron sputtering and explore the phase space of sample composition, growth temperature, post-annealing process, as well as resorting to suitable substrates and crystalline buffer layers. The samples are structurally characterized by a combination of X-ray diffraction and atomic-scale high-resolution transmission electron microscopy, which reveals a thickness-dependent microstructure of the B20 films, attributable to a combination of strain relaxation and the formation of extended defects, which are under detailed investigation. [1] B. Bradlyn et al., Science 353 (2016).[2] D. S. Sanchez, et al., Nature 567 (2019).[3] Z. Rao et al., Nature 567 (2019).

DS 4.2 Mon 16:45 REC/C213

high-quality Bi_2Te_3 TI thin films on [0001]-oriented sapphire substrate grown by MBE — •Ismet Gelen, Ahmet Yagmur, Luke Benson, and Satoshi Sasaki — School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

Over the past decades, topological insulators (TIs) have attracted great attention for their exotic property of being insulating in the bulk while conductive on the surfaces through topological surface states [1], offering promising prospects for future spintronic technologies [2]. Molecular beam epitaxy (MBE) growth method is very important to produce high-quality epitaxial thin film TIs samples. However, producing a high-quality thin film requires careful consideration of substrate preference, growth temperature, and growth rate. This study focuses on the systematic growth of high-quality Bi_2Te_3 TI thin films on a sapphire [0001] substrate with minimal lattice mismatch. We found that growth temperature has a big influence on the surface morphology, which can lead to small or large triangular terraces. When temperature is too low it can create pillars when it is too high it creates defects/holes in films. We will report our optimization of the Bi_2Te_3 growth in terms of X-ray reflectivity/diffraction, atomic force microscopy, Raman spectroscopy, and magnetotransport properties by measuring standard Hall-bar type devices at low temperatures. Finally, we obtain films with large grain size without defects/pillars, and with high mobility and low carrier density.

[1] Li, Y., et al. (2022). ACS Nano, 16(6), 9953-9959. [2] Hasan, M. Z., et al. (2010). Reviews of Modern Physics, 82(4), 3045-3067.

DS 4.3 Mon 17:00 REC/C213

exploring ehalgogenide ABX3 perovskites: challenges and insights from physical vapor deposition — •Sebastian Zimmermann[1], Roland Scheer[2], and Torsten Hölscher[1] — [1]B5 Photovoltaics, Just Transition Center, Martin Luther Universität Halle-Wittenberg — [2]Photovoltaics Groups, Martin-Luther-Universität Halle-Wittenberg

The discovery of new solar cell materials is crucial for the next generation of multijunction systems in photovoltaics. This work focuses on synthesizing thin-film materials that are theoretically well suited for photovoltaic applications. To form these materials, we use physical vapor deposition (PVD). At the beginning, we aim to synthesize chalcogenide perovskites. Chalcogenide perovskites are crystals with a perovskite structure (typically ABX3), where X stands for selenium or sulfur, A for group II metal like Ca or Ba and B for a transition metal like Ti or Zr. Compared to other perovskites, their advantages include lower toxicity and the predicted long-term stability of the layers. This talk presents results of microstructural analysis of PVD synthesized chalcogenide perovskite films and discuss challenges encountered during synthesis. Our results provide new insights in the field of photovoltaic materials and are intended to open up new perspectives for multijunction thin-film solar cells.

15 min. break

DS 4.4 Mon 17:30 REC/C213

Molecule Adsorption at Me-polar and N-polar 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 structures. The most important ones 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. Two different substrates were used to achieve either Me-polar (SiC) and N-polar (sapphire) wz-ScGaN surfaces. The interaction of gas molecules (oxygen and water) in vacuum were analyzed by X-ray (XPS) and ultraviolet photoelectron spectroscopy (UPS).

DS 4.5 Mon 17:45 REC/C213

Molecular Beam Epitaxy of ferrimagnetic Mn_4N — •Adriano Notarangelo, Michael Hanke, Lutz Geelhaar, Oliver Brandt, and Philipp M. John — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany.

Mn_4N is a ferrimagnetic transition-metal nitride that crystallizes in the anti-perovskite structure. With its strong perpendicular magnetic anisotropy and high Curie temperature of $\approx$ 743 K, Mn_4N emerges as a promising material for rare-earth-free spintronics and other magnetic device applications. Since the magnetic properties of Mn_4N are sensitive to stoichiometry, strain, and lattice defects, achieving high-quality epitaxial growth is essential.

In this work, we grow 60 nm–thick Mn_4N layers by plasma-assisted molecular beam epitaxy on sub-1% lattice-mismatched $SrTiO_3(001)$ substrates. After carefully calibrating the Mn/N flux ratio to achieve a 4:1 stoichiometric balance, we obtain phase-pure $Mn_4N(001)$ films with no detectable secondary Mn_xN_y phases. X-ray diffraction reveals that optimal crystalline quality is achieved for growth temperatures between 300 and 400°C, while substantial Mn desorption hinders growth above 600°C. The out-of-plane lattice constant decreases from 3.854 to 3.828 Å as the growth temperature increases from 300 to 500°C, indicating an increased in-plane tensile strain imposed by the epitaxial constraint to $SrTiO_3$ with its larger lattice constant.

The optimization of Mn_4N film growth on $SrTiO_3$ is a solid basis for its growth on industry-relevant substrates such as Si, SiC, and GaN.

DS 4.6 Mon 18:00 REC/C213

Investigations of cubic boron nitride nucleation using in situ RHEED during pulsed laser deposition — •Falko Jahn, Laura Dienelt und Steffen Weissmantel — Laserinstitut Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida

Due to its outstanding properties such as second-highest hardness, the cubic allotrope of boron nitride (c-BN) has attracted significant interest from both academia and industry for decades. So far, challenges in the thin film deposition of this material have prevented a successful industrial application, for example as a wear-resistant coating for cutting tools. Although pulsed laser deposition (PLD) has enabled progress in this particular field, several aspects of the film formation process remain insufficiently understood. In particular, the process of nucleation from the hexagonal to the cubic phase still contains unanswered questions. In this work, the microstructure of the growing film is characterized in situ using reflection high-energy electron diffraction (RHEED). This enabled further insight into the nucleation process. The results provide support for the nucleation model of subplantation. These findings contribute to a deeper understanding of c-BN nucleation during PLD or similar PVD techniques.

DS 5: Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)

Time: Tuesday 9:30–10:45 Location: HSZ/0105

Invited Talk DS 5.1 Tue 9:30 HSZ/0105

Simulating high-temperature superconductivity in a triangular moiré lattice — •Kin Fai Mak — Luruper Chaussee 149 Bldg. 900 (MPSD), 22761 Hamburg, Germany

Moiré materials built on transition metal dichalcogenide semiconductors have emerged as a tunable platform for simulating the Hubbard model on a triangular lattice. A natural question arises: Can the platform be tuned to yield a phase diagram similar to that in high-temperature cuprate superconductors? In this talk, I will discuss the emergence of high-temperature superconductivity near the Mott transition in a triangular moiré lattice with intermediate coupling strength. The emergent doping-temperature phase diagram looks remarkably similar to that in cuprate superconductors. I will also discuss the evolution of the phase diagram by tuning the band structure of the material by gating. The results could provide a new angle for understanding the phenomenon of high-temperature superconductivity in strongly correlated materials.

DS 5.2 Tue 10:00 HSZ/0105

Engineering Hubbard models with gated two-dimensional moiré systems — •Yiqi Yang[1], Yubo Yang[2], Miguel Morales[3], and Shiwei Zhang[3] — [1]Lund University, Lund, Sweden — [2]Hofstra University, New York, USA — [3]Flatiron Institute, New York, USA

Lattice models are powerful tools for studying strongly correlated quantum many-body systems, but their general lack of exact solutions motivates efforts to simulate them in tunable platforms. Recently, a promising new candidate has emerged for such platforms from two-dimensional materials. A subset of moiré systems can be effectively described as a two-dimensional electron gas (2D EG) subject to a moiré potential, with electron-electron interactions screened by nearby metallic gates. In this talk, we present the realization of lattice models in such systems [1]. We show that, by controlling the gate separation, a 2D EG in a square moiré potential can be systematically tuned into a system whose ground state exhibits orders analogous to those of the square lattice Hubbard model, including the stripe phase. Furthermore, we study how variations in gate separation and moiré potential depth affect the ground-state orders. A number of antiferromagnetic phases, as well as a ferromagnetic phase and a paramagnetic phase, are identified.We then apply our quantitative downfolding approach to triangular moiré systems closer to current experimental conditions, compare them with the square lattice parameters studied, and outline routes for experimental realization of the phases.
[1] arXiv:2508.13314

DS 5.3 Tue 10:15 HSZ/0105

Dirac quantum criticality in twisted double bilayer transition metal dichalcogenides — •Jan Biedermann and Lukas Janssen — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

We investigate the phase diagram of twisted double bilayer transition metal dichalcogenides with ABBA stacking as a function of twist angle and pressure. At a filling of 2 holes per moiré unit cell, the noninteracting system hosts a Dirac semimetal with graphene-like low-energy bands. At small twist angles however, interactions dominate the low-temperature physics, stabilizing an antiferromagnetic insulating ground state that is characterized by spin density modulations at the moiré scale. The twist-tuned semimetal-to-antiferromagnet transition is shown to be continuous and belongs to the Gross-Neveu-Heisenberg universality class. We propose that this transition may also be realized by applying uniaxial pressure to a sample, raising the intriguing possibility of experimentally measuring the associated critical exponents for the first time.

DS 5.4 Tue 10:30 HSZ/0105

Chemically Tunable Correlation Strength in Breathing Mode Kagome van der Waals Materials $Nb_3(F,Cl,Br,I)_8$ — •Joost Aretz[1], Sergii Grytsiuk[1], Xiaojing Liu[2], Giovanna Feraco[2], Chrystalla Knekna[2,3], Muhammad Waseem[2], Zhiying Dan[2], Marco Bianchi[4], Philip Hofmann[4], Mazhar Ali[5], Mikhail Katsnelson[1,6], Antonija Grubišić-Čabo[2], Hugo Strand[7], Erik van Loon[8], and Malte Rösner[1,9] — [1]Radboud University, Nijmegen, Netherlands — [2]University of Groningen, Netherlands — [3]University of Amsterdam, Netherlands — [4]Aarhus University, Denmark — [5]Delft University of Technology, Netherlands — [6]Constructor University, Bremen, Germany — [7]Örebro University, Sweden — [8]Lund University, Sweden — [9]Bielefeld University, Germany

Finding tunable correlated electron systems in nature is highly desirable for studying strongly correlated materials. Our recent work demonstrates that the Nb_3X_8-family offers such a platform for tuning correlation effects in van der Waals systems. By using ab initio downfolding and cluster dynamical mean-field theory we show how correlation effects evolve across the halide series. In these materials an intruiging interplay between in-plane trimerization and out-of-plane dimerization leads to correlated insulating behavior, where the strength of correlations can be tuned by switching the halide or by changing the layer number. The predicted trends are supported by ARPES measurements. The correlated electron physics in this system is robust, tunable and layered, which allows studying the role of correlations in devices such as the $NbSe_2/Nb_3Br_8$ Josephson diode.

DS 6: Thin Oxides and Oxide Layers

Time: Tuesday 9:30–11:45 Location: REC/C213

Invited Talk DS 6.1 Tue 9:30 REC/C213

Soft X-ray Microscopy of Ferroic Thin Films — •Tim A. Butcher[1], Simone Finizio[2], Michael Schneider[1], Jörg Raabe[2], Stefan Eisebitt[1], and Bastian Pfau[1] — [1]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany — [2]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Any technological advance involving ferroic thin films requires a clear picture of their domain structures at the nanoscale. These can be studied by soft X-ray microscopy at synchrotron lights sources, which combines high spatial resolution with sensitivity to ferroic order. This presentation will provide an overview of several ferroic thin films and the application of coherent diffractive imaging methods such as Fourier Transform Holography and soft X-ray ptychography to their study [1]. One example is the room-temperature multiferroic BiFeO3 for which ptychography can probe the magnetoelectric coupling by resolving both the antiferromagnetic spin cycloid and the ferroelectric domains in a single measurement [2,3]. Furthermore, an example of imaging dynamics will be provided with the ptychographic investigation of magnetic domain walls [4].

[1] T. A. Butcher et al., Rev. Sci. Instrum. 96, 123704 (2025) [2] T. A. Butcher et al., Adv. Mater. 36 (2024) [3] T. A. Butcher et al., Phys. Rev. Appl. 23, L011002 (2025) [4] T. A. Butcher et al., Phys. Rev. B 111, L220409 (2025)

DS 6.2 Tue 10:00 REC/C213

Atomic Scale Insights into the Polymorphism of Ruddlesden-Popper Nickelates and Titanates — Shihao Wei[1], Stefania Baronio[2], Bruce Davidson[2], Ke Zou[2], and •Nicolas Bonmassar[1] — [1]Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenberstr. 3, 70569, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Ruddlesden-Popper (RP) oxides provide an ideal platform for investigating coupled structural and electronic phenomena, as subtle variations in layering and cation coordination can significantly alter their functional properties. Using oxide molecular beam epitaxy, we can grow distinct nickelate and titanate RP phases with atomic-layer precision, demonstrating the controlled stabilization of distinct polymorphs

by tuning the rock-salt and perovskite layers. Advanced scanning transmission electron microscopy provides insights into the resulting structures at an atomic scale, enabling the direct identification of the respective polymorph and the characterization of extended defects, such as stacking faults. By correlating local structure with electronic properties, we can establish clear structure-property relationships across all samples. Electron energy-loss and energy-dispersive X-ray spectroscopy reveal the differences in transition-metal oxidation states, defect density and oxygen orbital occupation between the different RP phases and polymorphs. Our results highlight how precise control of the individual layers leads to the control over the polymorphs in RP nickelates and titanates.

DS 6.3 Tue 10:15 REC/C213

Memristive behaviour in Nickelate Perovskite thin films — •Foelke Janssen[1,2] and Beatriz Noheda[1,2] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, The Netherlands

Memristive devices can adopt multiple resistance states depending on the history of the electric signal applied, emulating the basic behavior of synapses and neurons. They hold great promise as low energy consumption devices for in-memory and brain-inspired computing. Materials that undergo a metal-to-insulator phase transition (MIT) are interesting as volatile memristors and can also be used as neuristors by being the active component in self-oscillating circuits. Rare-earth (RE) nickelates ($RENiO_3$) display a MIT at temperatures that can be tuned by changing the RE cations, the strain state, the film thickness or the oxygen vacancy content. Compared to other transition-metal oxides, nickelates are especially interesting as memristive devices due to the robustness of the perovskite structure under intense local heating. In this work, we demonstrate that nickelates can also be used to mimic short term memory in synapses via multilevel resistance states that can be achieved in $SmNiO_3$ thin film structures upon voltage pulsing, harnessing the metal-insulator phase transition, without involving ionic transport. Furthermore, we also demonstrate $SmNiO_3$ as a neuron and discuss the mechanisms behind both devices.

15 min. break

DS 6.4 Tue 10:45 REC/C213

Structure and optical properties of Ga2O3 thin films deposited by reactive and non-reactive sputtering — •Marcell Gajdics, Ildikó Cora, Dániel Zámbó, Zsolt Endre Horváth, Miklós Serényi, and Béla Pécz — Institute for Technical Physics and Materials Science, HUN-REN Centre for Energy Research, H-1121 Budapest, Hungary

Ga2O3, as an ultrawide bandgap semiconductor has numerous potential applications in the field of optoelectronics and high-power electronics. Gallium oxide thin films can be grown by a variety of methods, among which radio frequency sputtering is a commonly used technique. In most cases, a ceramic Ga2O3 target is used for the sputter deposition of Ga2O3. In our work, we present an alternative method, i.e. reactive sputtering of a liquid Ga target. We have shown that by using this technique, layers close to the ideal stoichiometry can be deposited with higher deposition rates than by using a Ga2O3 target. The optical properties (e.g. refractive index) were studied as a function of the oxygen concentration in the films. Post-deposition annealing experiments were also performed on the amorphous as-deposited layers to study the annealing-induced structural and optical changes. It was found that as a first step of crystallization γ-Ga2O3 phase was formed and the thermodynamically stable β-Ga2O3 appeared only at higher temperatures. The photoluminescence emission and the optical bandgap were also measured at different annealing temperatures and the results were correlated with the structural properties.

DS 6.5 Tue 11:00 REC/C213

Depth Profiling of Oxygen Migration in Ta/HfO_2 Stacks During Ionic Liquid Gating — •Martin Wortmann[1,2], Beatrice Bednarz[3], Olga Kuschel[3,4], Fabian Kammerbauer[3], Mathias Kläui[3], Andreas Hütten[1], Joachim Wollschläger[4], Gerhard Jakob[3], and Timo Kuschel[1,3] — [1]Bielefeld University, Bielefeld, Germany — [2]Bielefeld University of Applied Sciences and Arts, Bielefeld, Germany — [3]Johannes Gutenberg University Mainz, Mainz, Germany — [4]Osnabrück University, Osnabrück, Germany

Ionic-liquid gating enables electric-field-driven ion transport at thin-film interfaces to manipulate structural, electronic, optical, and magnetic properties [1]. Oxygen is driven from a donor oxide layer into an underlying acceptor metal layer, but the resulting spatial distribution and voltage dependence of oxygen migration remain poorly understood. Here, we investigate the formation of Ta_2O_5 at the interface between the HfO_2 donor and Ta acceptor layers as a function of gate voltage, time, and HfO_2 thickness using oxidation-state depth profiling by combining X-ray reflectivity measurments with multi-line angular-resolved X-ray photoelectron spectroscopy [2,3]. The results elucidate both the quantitative oxygen distribution as well as the underlying mechanism [4].

[1] Bednarz et al., Appl. Phys. Lett. 124, 232403 (2024)
[2] Wortmann et al., Small Methods 8, 2300944 (2023)
[3] Wortmann et al., Appl. Surf. Sci. 713, 164356 (2025)
[4] Bednarz et al., arxiv: 2509.05748 (2025)

Invited Talk DS 6.6 Tue 11:15 REC/C213

Charge transfer at interfaces of free-standing oxide membranes and heterostructures — Kapil Nayak[1], Lee-Kang Huang[1], Anton Kaus[1], Marcus Wohlgemuth[1], Alexandros Sarantopoulos[1], Christoph Baeumer[2], Regina Dittmann[1], and •Felix Gunkel[1,2] — [1]PGI-7, FZ Jülich — [2]MESA+, UTwente

Free-standing oxides, based on the delamination of atomically defined epitaxial thin films, provide new opportunities to combine functional complex oxides with semiconductor electronics and other typically incompatible technology environments. The nanoscale confinement of these transferable membranes enables unique structures and functionalities, applicable in hybrid electronics as well as energy applications. Here, we discuss the synthesis of transferable perovskite oxide membranes and heterostructures via the all-perovskite sacrificial-layer route. We present control strategies to achieve singly-terminated membranes, using chemical treatments as well as direct growth mode control. These yield atomically smooth membrane-based substrates, serving as ideal template for heterostructure growth on Si. We use typical charge-transfer oxide heterostructures, such as LaAlO3/SrTiO3, to probe the interfacial charge-transfer across the heterostructure interface. To disentangle growth-induced redox response and thermodynamic ion-exchange, we employ in-situ x-ray spectroscopy and correlate the interplay of confinement-phenomena, redox-chemistry & growth kinetics. Finally, we will provide an outlook on membrane-based oxide heterostructures used in electrochemical water splitting, offering new opportunities for analysis and integration.

DS 7: Thermoelectric and Phase Change Materials

Time: Tuesday 10:00–11:30 Location: REC/B214

DS 7.1 Tue 10:00 REC/B214

Voltage-Controlled Magnetism via Electrically Triggered Metal-Insulator Transitions — •Lorenzo Fratino — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université

Phase separation is key to understanding magnetism in correlated systems like manganites. This talk will show how the resistive switching in metal-insulator transition (MIT) materials can be used to create and control artificial phase separation with voltage. In (La,Sr)MnO*, a threshold voltage triggers an electrothermal MIT, creating a paramagnetic insulating barrier inside a ferromagnetic metallic matrix [1]. We can use this to directly tune magnetic properties, achieving effects like voltage-triggered magnetic anisotropy switching [2]. We also developed a CdS/LSMO heterostructure where light injection modulates resistance drop*comparable to a 9 T magnetic field, while surprisingly decoupling the optical and magnetic responses [3]. This work establishes a versatile pathway for voltage-controlled magnetism using MIT materials [4].

References: [1] Nat. Commun. 12, 5499 (2021) [2] Phys. Rev. B 108, 174434 (2023) [3] Phys. Rev. Appl. 19, 044077 (2023) [4] Adv. Funct. Mater. 2419840 (2025)

DS 7.2 Tue 10:15 REC/B214

Thermoelectric power factors of defective scandium nitride nanostructures from first principles — •Luigi Cigarini[1], Urszula D. Wdowik[1], and Dominik Legut[1,2] — [1]IT4Innovations, VŠB Technical University of Ostrava, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

In scandium nitride (ScN), structural defects and chemical impurities strongly affect thermoelectricity (TE), although transport mechanisms remain unclear [1-3]. Reported electronic transport in ScN thin films shows large variability, and strategies to enhance TE efficiency often yield conflicting results [4,5]. Here, using the Landauer approach, we analyze how different types of imperfections affect electronic transport in ScN lattice. Defects are classified according to their symmetry (isolated, multiple contiguous, involving stacking mismatches) and chemical nature (oxygen impurities, nitrogen-site vacancies). Our theoretical results identify two dominant defect classes with opposing effects on TE performance: (i) contiguous nitrogen vacancies, which enhance el. conductivity but reduce the magnitude of the Seebeck coeff. (S), and (ii) oxygen substitutions coupled with nearby stacking mismatches, which increase the magnitude of S while hindering el. conductivity. In this way, we propose a rationale that relates part of the experimental variability to its microscopic origin [6]. [1] Phys. Rev. Mater. 3, 020301 (2019), [2] J. Mater. Chem. C 4, 3905 (2016), [3] Phys. Rev. B 86, 195140 (2012), [4] J. Appl. Phys. 113, 153704 (2013), [5] Appl. Surf. Sci. Adv. 25, 100674 (2025), [6] Preprint: arXiv:2509.14762.

DS 7.3 Tue 10:30 REC/B214

Understanding Charge Transport in ZnO Quantum Dots Through Combined Thermoelectric and High-Field Measurements — •Henrik Holzhauser, Morteza Shokrani, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

ZnO Quantum Dot (QD) solids are an attractive material for a wide range of applications. ZnO QDs also make an excellent model system for QD solid in general owing to the ability to tune the effective diameter of ZnO QD via UV illumination, and the effective electronic localization length via ligands. The charge transport in QD solids is typically explained as thermally activated tunnelling or hopping between the localized states of individual QDs. As such, the electric conductivity is both electric field and temperature dependent. In comparison, the Seebeck effect in QD solids, especially in connection with the electrical conductivity, is not as precisely understood. Here, we combine measurements of the Seebeck coefficient for various ZnO QDs with electric field- and temperature-dependent conductivity measurements, all performed at lattice temperatures ranging from 100 to 300K. We used bare ZnO QDs and ZnO QDs with ligands of various lengths and measured all QD solids at multiple UV-induced effective diameters. The wide range of experiments allows us to obtain a comprehensive understanding of the dominant mechanisms and the characteristic energy and length scales in the system. We find that transport is dominated by energetic disorder resulting from a diameter-dependent charging energy, in combination with an effective localization energy that reflects both wavefunction decay and morphology.

15 min. break

DS 7.4 Tue 11:00 REC/B214

Classification of Metal - Insulator Transitions: Insights from characteristic Property Changes and related Quantum Mechanical Bonding Descriptors — •Tim Bartsch[1], Raagya Arora[4], Carl-Friedrich Schön[1], Umesh Waghmare[3], 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 — [3]Theoretical Sciences Unit, School of Advanced Materials JNCASR Jakkur, Bangalore 560064, India — [4]John A. Paulson School of Engineering and appled science, Havard University, Cambridge Massachusetts

The nature of the transition between metals and insulators is one of the most fascinating topics in condensed matter physics. The end points of this transition are well-defined, i.e. a solid which has a non-vanishing electrical conductivity σ in the limit T * 0 K is a metal, while an insulator is characterized by σ = 0 S/m (T * 0 K). In 1980, Rosenbaum and co-workers investigated the metal-insulator transition in phosphorus-doped silicon, by measuring the low-temperature resistivity of samples with different doping concentrations. Here, we are pursuing a rather different goal. We are looking at a range of different crystalline insulators and check whether they can be classified as pressure-controlled MITs based on characteristic changes in their properties. Such pressure-driven MITs occur in all insulating solids at sufficiently high pressures when the orbital overlap of neighboring atoms increases sufficiently to favor a metallic state.

DS 7.5 Tue 11:15 REC/B214

Effect of Ge doping and thickness on anomalous Nernst effect in Fe4N thin films — •Robin K. Paul[1], Jakub Vít[2], Karel Knížek[2], Petr Levinský[2], Ondřej Kaman[2], Mariia Pashchenko[2], Lenka Kubíčková[2], Kyo-Hoon Ahn[2], Markéta Jarošová[2], Joris More-Chevalier[2], Stanislav Cichoň[2], Tomáš Kmječ[3], Jaroslav Kohout[3], Marcus Hans[4], Stanislav Mráz[4], Jochen M. Schneider[4], Giovanni d'Andrea[1], Lambert Alff[1], Esmaeil Adabifiroozjaei[1], Leopoldo Molina-Luna[1], Oliver Gutfleisch[1], and Imants Dirba[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Institute of Physics of the CAS, Praha, Czech Republic — [3]Charles University, Praha , Czech Republic — [4]RWTH, Aachen, Germany

Anomalous Nernst Effect(ANE)-based devices have recently emerged as a promising alternative to Seebeck based ones, offering simpler geometries. However, their adoption is constrained by lower efficiencies compared to Seebeck-based counterparts. This study focuses on exploring materials with high ANE coefficients. Among the candidates, Fe_4N has attracted attention due to its cost-effectiveness, and tunability through elemental doping. DFT calculations indicate that doping Fe_4N with Ge can enhance its ANE coefficient. In this work, thin films of doped $Fe_{4-x}Ge_xN$ were fabricated onto MgO substrates. The evolution of crystal structure and microstructure are systematically characterized correlating with Nernst effect. ANE is also reported to increase with decrease in film thickness which was investigated by preparing Fe_4N films of thickness from 5nm to 50nm.

DS 8: Transport Properties

Time: Tuesday 14:00–15:30 Location: REC/B214

DS 8.1 Tue 14:00 REC/B214

Polaron Transport in $BiVO_4$ — •Nils Sekinger[1,2], Tsedenia Zwedie[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University Munich — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich

Bismuth vanadate ($BiVO_4$) has received considerable attention as a potential photoanode for photocatalytic applications, thanks to its moderate bandgap of ∼2.5 eV and favourable band edge energetics. However, it is believed that photogenerated electrons localise at vanadium sites to form small polarons, while holes localise around BiO_8 units to form large polarons, thereby inhibiting their transport [1]. This study investigates charge transport in monoclinic $BiVO_4$ using temperature-dependent photoconductivity measurements. Under illumination, we observe two distinct thermally-activated transport regimes. With decreasing temperature, the large-barrier electron hopping transport characteristic transitions to a lower barrier regime that may arise from the freeze-out of electron transport, resulting in a dominant influence from minority holes. The transport barriers, hopping distances, and effective masses of both small and large polarons in the dark and with illumination at different intensities are investigated. Analysing the dependence of the resistivity on temperature and light intensity provides critical insights into the polaronic conduction mechanism and offers experimental validation for theoretical models describing polaron transport. These findings improve our understanding of charge transport in $BiVO_4$ and its use in photocatalytic and electrochemical applications.

[1] *Wiktor et al. ACS Energy Lett. 2018, 3(7), 1693-1697*

DS 8.2 Tue 14:15 REC/B214

Correlation of impedance and structural properties in oxides on the microscale — •Jan L. Dornseifer[1,2], Christopher P. Körbächer[1,2], Martin Becker[1,2], Janis K. Eckhardt[2], Matthias T. Elm[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Jusuts-Liebig-University Giessen, Germany

The charge transport properties of ionically and/or electronically conducting thin films are governed by their elemental composition and microstructure, including their morphology and grain architecture. Electrochemical impedance spectroscopy (EIS) is widely used to probe the electrical properties, yielding macroscopic parameters. However, linking these to the underlying microscopic transport processes requires theoretical models that have so far failed for samples with expansions comparable to their grain sizes.

Here, we present an experimental approach to directly relate impedance, microstructure and microscopic transport properties. Using cerium oxide and vanadium oxide networks with well-defined microscale transport paths, the impedance of individual networks was measured via microelectrodes. Complementary SEM, EDX, and micro-Raman spectroscopy provided detailed structural information. Correlating these data with the impedance offered new insights into the microstructural influences on the charge transport. This represents a promising way to reliably determine microscopic transport properties of polycrystalline thin films on the microscale.

DS 8.3 Tue 14:30 REC/B214

Magnetotransport and Electron Optics in Bilayer Graphene — •Florian Schöppl[1], Ming-Hao Liu[2], Alina Mrenca-Kolasinska[3], Klaus Richter[1], Korbinian Rohrmüller[1], Korbinian Schwarzmaier[1], and Angelika Knothe[1] — [1]Institut für Theoretische Physik, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan City, Taiwan — [3]AGH University of Krakow, Kraków, Poland

The remarkable sample quality of bilayer graphene (BLG), combined with the strong electrostatic tunability of its band structure, makes BLG an excellent platform for electron optics. While the system's purity enables ballistic transport on micrometer scales [1,2], trigonal warping near each K point induces a valley-dependent momentum selection, resulting in characteristic anisotropic transport and scattering phenomena [3,4]. To study the interplay between such warping effects and symmetry breaking from gate-defined potentials, we employed quantum-mechanical tight-binding models as well as semiclassical simulations and find pronounced directional conductance in BLG cavities. Motivated by these anisotropic properties, we further analyze unguided -ringless- Aharonov-Bohm configurations and used wave-matching algorithms to tailor electrostatically defined lenses [5] and mirror geometries.

[1] L. Seemann et al., Phys. Rev. B (2023) [2] L. Banszerus et al., Nano Lett. 2016 [3] C. Gold et al., Phys. Rev. Lett. (2021) [4] J. K. Schrepfer et al., Phys. Rev. B (2021) [5] C. G. Péterfalvi et al., New J. Phys. 14 (2012)

15 min. break

DS 8.4 Tue 15:00 REC/B214

Multiscale Simulation of Charge Transport Across Grain Boundaries in Organic Polycrystalline Thin-Film Semiconductors — •Junior-Wilfried Tadjeugue-Nangmo[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Grain boundaries (GBs) are known to critically limit charge carrier mobility in organic polycrystalline semiconductors as already used in e.g. organic field effect transistors. In our contribution, we address Technologies with a multiscale computational framework that correlates a GB's morphology with its influence on the charge transport properties. Our approach is, at its core, based on phase-field simulations of grain growth to generate realistic GB networks. Electronic structure calculations then reveal deep trap states and significant energetic disorder at the GB, leading to substantial injection barriers. Charge transfer rates across GBs are then calculated from a hopping model which are finally fed into kinetic Monte Carlo (KMC) simulations to demonstrate the device level influence of GBs. They elucidate the fundamental role of grain boundaries in limiting charge transport and provide critical guidelines for the development of future high-performance organic electronics devices.

DS 8.5 Tue 15:15 REC/B214

Modeling of Indium Tin Oxide Back Contacts in CIGSe Solar Cells — •Oliver Wolf[1], Merve Demir[2], Matthias Maiberg[2], Torsten Hölscher[1], and Roland Scheer[2] — [1]B5 Photovoltaics, Just Transition Center, Martin Luther University Halle-Wittenberg — [2]Photovoltaics Group, Martin Luther University Halle-Wittenberg

Copper Indium Gallium Diselenide (CIGSe) thin-film solar cells achieve high efficiencies >23% on opaque molybdenum (Mo) back contacts (BC). Substituting the molybdenum by a transparent conductive oxide, such as Indium Tin Oxide (ITO), facilitates applications in tandem solar cells or bi-facial configurations, but leads to deteriorated Fill Factors and Open-Circuit Voltages. The origin of the inferior solar cell performance remains unclear, but impeded electronic transport at the rear CIGSe/ITO interface appears most likely, especially in view of thin Gallium Oxide interlayers. To elucidate possible transport mechanisms, temperature-dependent current-voltage (JVT) and capacitance-frequency (CfT) characteristics were performed and analysed by means of numerical simulations with Sentaurus from Synopsys. In the measurements, we observe the occurrence of temperature-dependent kinks in the JVT and steps in CfT, which clearly distinguish the measurements of the solar cells with ITO BC from those with Mo. Based on simulation, tunneling processes turn out to be the dominant transport mechanism at the rear interface. Our results are able to describe the observed performance deficits in CIGSe solar cells with ITO BC.

DS 9: Thin Film Properties III: Oxides

Time: Tuesday 14:00–15:15 Location: REC/C213

DS 9.1 Tue 14:00 REC/C213

Analysis of the MgF_2 || VO_2 Interface in Applications as Smart Windows by Secondary Ion Mass Spectrometry (SIMS) — •Yan Ravil Wollenweber-Bienerth, Peter J. Klar, Anja Henss, and Martin Becker — Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany

Smart Windows are special fenestration devices whose transmittance switches as a function of the ambient temperature. Vanadium dioxide (VO_2) is by far the most studied material for such applications. Usually, high substrate temperatures are needed to obtain VO_2 thin films. This results in detrimental diffusion of alkaline ions from the substrate into the thermochromic layer. Buffer layers between the substrate and the VO_2 may prove a suitable option for reducing this effect. Additionally, these help to increase visible transmittance and, in case of rutile materials, yield a reduction of the VO_2 growth temperature. Magnesium fluoride (MgF_2) is one viable candidate thanks to its excellent optical properties and chemical resistance. Simulations, however, show a significant influence of the interfaces between the layers on various properties. By controlling interface morphology, an improvement of the layer properties can be anticipated.

Here, we utilize SIMS depth-profiling to analyze multi-layer stacks of VO_2 and MgF_2 grown by ion-beam sputter deposition (IBSD). The stacks werde deposited on quartz glass substrates with MgF_2 serving as buffer layer. We show that this type of buffer layer improves the layer properties.

DS 9.2 Tue 14:15 REC/C213

Modification of crystal structure of TiO_2 thin films for artificial photosynthesis — •Lauri Palmolahti — University of Würzburg, Würzburg, Germany — Tampere University, Tampere, Finland

Progressing climate change has created a need for carbon-neutral energy production methods, such as artificial photosynthesis. The corrosive nature of artificial photosynthesis requires the use of coatings to protect otherwise unstable photocatalytic materials. The crystallite structure and size significantly affect the protective properties and chemical stability of the thin film. In this work, the effect of defect composition in amorphous TiO_2 thin films on vacuum annealing induced crystallization was studied. The chemical stability and protective properties of these crystallized films were then examined under conditions similar to those in artificial photosynthesis. The defect composition of the amorphous phase, such as Ti^{3+}, O^{1-}, and precursor traces, was tuned by changing the deposition parameters. The results showed that amorphous TiO_2 thin films without Ti^{3+} defects crystallized into microcrystalline anatase, whereas a moderate number of these defects led to the formation of nanocrystalline rutile. An excessive number of defects resulted in a mixed amorphous–nanocrystalline rutile phase. Impedance spectroscopy and stability tests revealed that microcrystalline anatase was prone to grain boundary corrosion, whereas nanocrystalline rutile was chemically stable and retained its protective properties for extended periods of time, making it a suitable choice for protective coatings in artificial photosynthesis.

DS 9.3 Tue 14:30 REC/C213

Investigation of epitaxial ITO layers on YSZ as a transparent conductive back contact for photoelectrochemical applications — •Margaretha Huber[1], Sergej Levashov[1], Tsedenia Zewdie[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]TUM School of Natural Sciences — [2]Walter Schottky Institut

Photoelectrochemical (PEC) water splitting is a promising route toward sustainable, high-energy-density solar fuels for carbon-neutral energy storage. Transparent conducting oxides such as indium tin oxide (ITO) often serve as back contacts due to their high electrical conductivity, electrochemical stability in the oxygen evolution reaction, and favorable band alignment. ITO grown on cubic oxide substrates such as yttria-stabilized zirconia (YSZ) can act as an epitaxial template with low lattice mismatch, enabling fully epitaxial oxide heterostructures with well-defined interfaces and reduced defect densities. Here, we investigate epitaxial ITO (100) thin films on YSZ grown by e-beam evaporation through a systematic variation of deposition rate, substrate temperature, and post-deposition annealing atmosphere, thereby tuning crystallinity, lattice parameters, carrier transport, and surface morphology. The correlation between structural quality and stoichiometry, and their impact on electrical properties, is investigated using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). These ITO/YSZ templates are evaluated using $BiVO_4$ as a model photoanode to enable efficient charge extraction and provide design guidelines for epitaxial oxide heterostructures for PEC water splitting.

DS 9.4 Tue 14:45 REC/C213

Room-temperature H_2 gas sensing in ultra-thin SnO_2 films grown via atomic layer deposition — •Rudi Tschammer[1], Dominic Guttmann[1], Carlo Tiebe[2], Karsten Henkel[1], Carlos Morales[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Transitioning to an energy system based entirely on renewable energy sources requires long-term energy storage utilizing energy vectors such as hydrogen (H_2). Given its high diffusivity, broad explosive range, and low ignition energy, the adoption of H_2 requires safety systems along the hydrogen value chain. Therefore, there is a need for sensitive, specific and selective conductometric H_2 sensors operating at room temperature (RT) and compatible with complementary metal-oxide semiconductor (CMOS) technology. Earlier work by our group investigated ultra-thin cerium oxide films grown by atomic layer deposition (ALD) and demonstrated H_2 sensing at RT. This performance was due to the abundant defects present in the films. Building on these results, we present a comprehensive investigation of ALD-grown tin oxide (SnO_2), a widely researched metal oxide for H_2 gas sensing. Using *in-situ* X-ray photoelectron spectroscopy (XPS), we observe a distinct dependence of defect concentration on film thickness and oxidant. *Ex-situ* H_2/air gas sensing measurements and near-ambient pressure XPS further link film properties and sensing behavior. These findings pave the way for novel RT H_2 gas sensors based on ALD technology.

DS 9.5 Tue 15:00 REC/C213

Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY, Hamburg

Beta-phase gallium oxide has a band gap of 4.85 eV, suggesting strong potential for high-power electronics applications. Its properties can be enhanced by increasing the band gap via aluminum alloying. Here, we discuss the structural, electronic, and surface properties of β-$(Al_xGa_{1-x})_2O_3$ bulk crystals and thin films grown by metal-organic vapor-phase epitaxy (MOVPE) with Al contents of up to 40 %. Their Al content was determined by X-ray photoelectron spectroscopy (XPS) and compared with values obtained from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, potential doping gradients towards the bulk have been investigated by acquiring spectra at different take-off angles and by XPS depth profiling, revealing different aluminum concentrations in the bulk and at the surface. Furthermore, we establish a correlation between Al content and electronic band gap, i. e., with changes in the optoelectronic properties, which were determined by a combination of XPS electron-loss spectra and optical absorbance measurements. Finally, Auger spectroscopy and XRD analysis confirm the excellent chemical and structural quality of β-$(Al_xGa_{1-x})_2O_3$ thin films.

DS 10: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)

Nickel, a direct neighbor of copper in the periodic table, has been considered a promising candidate for high-temperature superconductivity since the early 1990s. After more than three decades of research, this prediction was confirmed with the discovery of superconductivity in nickelates, marking the beginning of the "nickel age" of superconductivity. Recent advances include Sm-based infinite-layer nickelates with transition temperatures approaching 40 K, as well as bilayer nickelates exhibiting superconductivity above 90 K under pressure and up to 60 K under compressive epitaxial strain. These results highlight the crucial roles of structural engineering, epitaxial strain, and precise synthesis control, and they open new frontiers for both fundamental understanding and materials design. This focus session aims to define key scientific challenges ahead, strengthen collaboration within Germany and Europe, and accelerate progress toward higher superconducting transition temperatures.

Coordinators: Marta Gibert (TU Wien), Mattias Hepting (MPI FKF Stuttgart), Ilya M. Eremin (Ruhr-University Bochum)

Time: Wednesday 9:30–12:45 Location: HSZ/0003

Topical Talk DS 10.1 Wed 9:30 HSZ/0003
Unconventional Superconductivity in Infinite-layer Samarium Nickelates — •Danfeng Li — City University of Hong Kong, Kowloon, Hong Kong SAR, China

Infinite-layer nickelates have emerged as a frontier platform for studying unconventional superconductivity beyond the cuprates. In this talk, I will present our recent advances on samarium-based infinite-layer nickelate thin films, which exhibit enhanced superconductivity and a mixed two- and three-dimensional superconducting character arising from strong coupling between rare-earth $5d$ and Ni $3d$ orbitals. I will further highlight our discovery of robust field-induced re-entrant superconductivity in heavily Eu-doped $Sm_{0.95-x}Ca_{0.05}Eu_xNiO_2$, where superconductivity suppressed at low fields re-emerges above 6 T and persists to 45 T. This exotic high-field state results from the interplay between NiO-plane superconductivity and Eu^{2+}-sublattice ferromagnetism, revealing a unique coexistence of magnetism and superconductivity within a single material system. These findings demonstrate how rare-earth-site engineering and magnetic-field tuning provide powerful routes for realising and manipulating high-temperature ferromagnetic superconductivity.
[1] M. Yang, H. Wang, J. Tang, J. Luo et al., arXiv:2503.18346 (2025).
[2] M. Yang, J. Tang, X. Wu, H. Wang et al., arXiv:2508.14666 (2025).

Topical Talk DS 10.2 Wed 10:00 HSZ/0003
Recent insights into infinite-layer nickelate heterostructures from x-ray spectroscopy — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Nickelates have emerged as an important class of materials for studying unconventional superconductivity. However, the exact cation concentrations and oxygen stoichiometry in infinite-layer nickelates are difficult to determine due to the complex synthesis process. This has so far prevented the clear experimental identification of the nickel valence electron configuration in the superconducting phase.

In my talk, I will discuss our recent x-ray spectroscopy studies on $NdNiO_x$-$SrTiO_3$ heterostructures [1] and $PrNiO_x$ thin films [2] at various intermediate stages of topotactic reduction with $x = 2 - 3$. We find that even the most reduced films do not exhibit a pure Ni^{1+}-$3d^9$ configuration. The quantitative analysis shows that there is an average of 1.35 holes in the nickel $3d$ states and superconducting samples have even higher values [2]. These results challenge previous findings regarding the doping range in which superconductivity occurs in infinite-layer nickelates. Variations between samples are attributed to a complex interplay of ordered, self-doped regions, interfacial reconstructions, and disorder occurring on different length scales in both the cation and anion sublattices.
[1] R. A. Ortiz et al., Phys. Rev. Materials 9, 054801 (2025).
[2] R. Pons et al., submitted (2025).

Topical Talk DS 10.3 Wed 10:30 HSZ/0003
Theory of infinite-layer nickelate superconductors — •Karsten Held — TU Wien, Austria

The discovery of superconductivity in infinite-layer nickelates [1] marked a new age of superconductivity: the nickel age. Using density functional theory, dynamical mean-field theory and dynamical vertex approximation (DΓA [2]), we successfully predicted [3] the phase diagram T_c vs. Sr-doping of $Nd_{1-x}Sr_xNiO_2$ with –for an unconventional superconductor– unprecedented accuracy with defect free films synthesized only 3 years later [4]. Also, the normal state spin spectrum well agrees with resonant inelastic x-ray spectroscopy (RIXS) [5] and the one-particle spectrum with angular-resolved photoemission spectroscopy (ARPES) [6], which both enter into the calculation of T_c. With this excellent agreement to later experiments, we can now with some confidence calculate the phase diagram of finite-layer nickelates [7] and predict that infinite-layer nickelates have a much higher T_c under 100GPa of pressure even without any chemical doping [8].

This work has been supported by the ERC project 101201037 and the FWF project I5398.
[1] D. Li et al., Nature 572, 624 (2019).
[2] G. Rohringer et al., Rev. Mod. Phys. 90, 25003 (2018).
[3] M. Kitatani et al., npj Quantum Materials 5, 59 (2020).
[4] K. Lee et al., Nature 619, 288 (2023).
[5] L. Si et al., Phys. Rev. Res. 6, 043104(2024).
[6] P. Worm et al., Phys. Rev. B 109, 235126 (2024).
[7] A. Hausoel et al., npj Quantum Mater. 10, 69 (2025).
[8] S. Di Cataldo et al., Nature Comm. 15, 3952 (2024).

15 min. break

Topical Talk DS 10.4 Wed 11:15 HSZ/0003
Disorder and distortions: what electrons tell us about nickelate superconductivity — •Berit H. Goodge — MPI-CPfS, Dresden, Germany

Recent realizations of superconductivity in both square-planar and bilayer Ruddlesden-Popper nickelates have opened a host of opportunities to explore fundamental questions of high-temperature superconductivity, while simultaneously posing unique synthetic challenges. Despite recent breakthroughs in sample synthesis, however, the highest quality thin films still pose immense challenges for investigation of fundamental characteristics, such as the pairing symmetry of the superconducting order parameter. Systematically introducing point-like disorder with high-energy electron irradiation consistently suppresses the superconducting transition, pointing towards a sign-changing order parameter in square-planar nickelates [1]. In parallel, epitaxial stabilization of superconductivity in bilayer nickelate thin films has opened the door to investigate local atomic structure and bonding environments. Leveraging the highest accessible spatial resolution and light-element sensitivity enabled by state-of-the-art multislice electron ptychography, we survey a series of bilayer nickelate thin films spanning a full series of tensile and compressive strain. We combine these experimental with strain-decomposed DFT calculations to investigate correlations between the observed atomic structure and superconductivity [2].
[1] Ranna et al., *PRL* 135, 126501 (2025).
[2] Bhatt et al., arXiv:2501.08204 (2025).

Topical Talk DS 10.5 Wed 11:45 HSZ/0003
Superconducting gap structure and bosonic mode in $La_2PrNi_2O_7$ thin films at ambient pressure — •Hai-Hu Wen — Hankou Rd. 22, Gulou, Nanjing, China

The recent discovery of high temperature superconductivity in nick-

elate systems has generated tremendous interests in the community. The core issue to understand the pairing mechanism is about the superconducting gap and its symmetry. We have successfully synthesized the superconducting thin films of $La_2PrNi_2O_7$ with $T_c{}^{onset} = 41.5$ K, and measured the superconducting tunneling spectra after we expose the superconducting layer by using the tip-excavation technique. The spectrum shows a two-gap structure with $\Delta_1 = 9$ meV, $\Delta_2 = 6$-8 meV, and fittings based on the Dynes model indicate that the dominant gap should have an s-wave structure with low anisotropy, this allows us to select the s^{+-}-pairing symmetry among the two possibilities s^{+-} and d-wave. Furthermore, a clear bosonic mode with energy $\Omega = 30 \pm 2$ meV is observed, which further supports a sign reversal gap[1]. Our results shed new light in understanding the mystery of superconductivity in bilayer nickelate superconductors.

Collaborators: Huan Yang, Ilya M. Eremin, Shengtai Fan, Mengjun Ou, Marius Scholten, Qing Li, Zhiyuan Shang, Yi Wang, Jiasen Xu

[1] S. Fan et al., arXiv: 2506.01788

DS 10.6 Wed 12:15 HSZ/0003

Investigation of Ruddlesden-Popper nickelates and the monolayer-trilayer polymorph using Raman spectroscopy — •Vignesh Sundaramurthy[1], Abhi Suthar[1], Pascal Puphal[1,2], Hasan Yilmaz[3], Masahiko Isobe[1], Matteo Minola[1], Bernhard Keimer[1], and Matthias Hepting[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]2^{nd} Physics Institute, University of Stuttgart, 70569 Stuttgart, Germany — [3]University of Stuttgart, Institute for Materials Science, Materials Synthesis Group, Heisenbergstraße 3, 70569 Stuttgart, Germany

Ruddlesden-Popper nickelates have attracted intense interest following the discovery of superconductivity in several members of the series, including bilayer $La_3Ni_2O_7$, trilayer $La_4Ni_3O_{10}$, and structural polymorphs composed of monolayer-bilayer or monolayer-trilayer (ML-TL) units. In this talk, we explore the phononic and electronic Raman responses of high-quality ML-TL single crystals and contrast them with those of the other nickelate phases, using samples with optimized oxygen content.

DS 10.7 Wed 12:30 HSZ/0003

Multiorbital density wave in the trilayer nickelate $La_4Ni_3O_{10}$ — Abhi Suthar[1], Vignesh Sundaramurthy[1], Matias Bejas[2], Congcong Le[3], Pascal Puphal[1], Pablo Sosa-Lizama[1], Masahiko Isobe[1], Peter A. van Aken[1], Y. Eren Suyolcu[1], Matteo Minola[1], Andreas P. Schnyder[1], Xianxin Wu[4], Bernhard Keimer[1], Giniyat Khaliullin[1], Andres Greco[2], and •Matthias Hepting[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]UNR-CONICET, Rosario, Argentina — [3]RIKEN, Saitama, Japan — [4]Institute of Theoretical Physics, Beijing, China

Ruddlesden–Popper nickelates exhibit high-temperature superconductivity closely intertwined with charge and spin density wave order. However, fundamental questions persist regarding the orbital character and symmetry underlying the density wave instabilities. Using polarized Raman scattering on trilayer $La_4Ni_3O_{10}$, we resolve characteristic phonon anomalies and a redistribution of electronic spectral weight across the density wave transitions. Momentum-selective electronic Raman responses, combined with multiorbital model calculations, reveal a density-wave–induced gap with incoherent, non-mean-field opening and contributions from both Ni-$d_{x^2-y^2}$ and d_{z^2} states [1]. These results reconcile conflicting experimental reports of the density wave gap and underscore its multiorbital character.

[1] A. Suthar *et al.*, arXiv:2508.06440 (2025).

DS 11: Layer Deposition

Time: Wednesday 9:30–11:45 Location: REC/B214

DS 11.1 Wed 9:30 REC/B214

Photo-Assisted Atomic Layer Deposition — •Paul Butler[1,2], Simon Wörle[1,2], Pengyu Hu[1,3], Manfred Stemplinger[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institut, Technische Universität München, 85748, Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technische Universität München, 85748, Garching, Germany — [3]Department of Electrical Engineering, TUM School of Computation, Information and Technology, Technische Universität München, 85748, Garching bei München, Germany

Atomic layer deposition (ALD) is a powerful technique for uniformly coating complex surfaces with thin films, though achieving lateral control remains one of its main challenges. This work demonstrates the implementation of visible-wavelength excitation to assist in the ALD process, thereby providing an opportunity for selective-area deposition using beam-shaping. We demonstrate that optical laser excitation can be used to assist in several ALD processes. An optical laser was used to selectively photo-assist the deposition of TiO_2 on gold as well as monolayer MoS_2 at low temperatures. The molecular precursors, titanium isopropoxide (TTIP) and ozone were used for the low-temperature deposition of TiO_2 on gold, while tetrakis(dimethylamido)titanium (TDMAT) and water were used for the deposition of TiO_2 on MoS_2. Photoexcitation is also shown to reduce the nucleation delay when $MeCpPtMe_3$ and ozone are used to deposit platinum films on Si and SiO_2 surfaces, using. Samples are characterized with spectroscopic ellipsometry and AFM before and after depositions, with in-situ ellipsometry during ALD procedures.

DS 11.2 Wed 9:45 REC/B214

Epitaxial growth of wurtzite $Al_{1-x}Hf_xN$ thin films by reactive magnetron sputtering — •Valentin Walbrunn[1,2], Laura I. Wagner[1,2], Verena Streibel[1,2], Mingyun Yuan[3], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Ternary nitrides such as transition metal (TM) wurtzite $Al_{1-x}TM_xN$ compounds offer great potential for future electromechanical and ferroelectric devices. While this class of materials is exemplified by $Al_{1-x}Sc_xN$, alternative TM elements such as Hf, Zr, and Ti remain largely underexplored, despite predictions of increased piezoelectric responses and the benefit of reduced reliance on rare earth elements. In this work, we explore reactive magnetron co-sputtering of wurtzite aluminum hafnium nitride ($Al_{1-x}Hf_xN$) to achieve epitaxial thin films suitable for high-frequency surface acoustic wave (SAW) applications. We tune the Hf content by scaling the power applied to the metallic Hf and Al targets in an Ar/N_2 atmosphere and determine optimized conditions with Hf cation fractions up to 40 %. X-ray diffraction confirms the formation of a wurtzite phase with strong c-axis orientation, and rocking curve measurements indicate improved crystalline quality, comparable to sputtered $Al_{1-x}Sc_xN$. These films demonstrate epitaxial wurtzite $Al_{1-x}Hf_xN$ as a promising material platform for high-frequency SAW applications.

DS 11.3 Wed 10:00 REC/B214

Epitaxial growth of hexagonal boron nitride (h-BN) by thermal laser epitaxy (TLE) — •Markus A. Blonski[1], Gideok Kim[2], João Marcelo Lopes[1], Audrey Gilbert[1], Lutz Geelhaar[1], Jochen Mannhart[2], Darrell G. Schlom[3], and Patrick Vogt[1,2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Cornell University, Ithaca, USA

Thermal laser epitaxy (TLE) is a novel thin film synthesis technique in which the substrate and sources are heated by high-power infrared lasers. Without heating elements, TLE achieves unprecedentedly high growth temperatures and pressures, exceeding those of traditional methods like standard chemical vapor deposition (CVD) or molecular beam epitaxy (MBE). TLE enables thermal in situ substrate termination, accelerating surface treatment and avoiding pre-growth contamination. Using TLE, we map an unrivaled growth pressure and temperature (P-T) parameter space for h-BN growth on $Al_2O_3(0001)$ substrates. To optimize substrate termination, the Al_2O_3 surface is nitridized to form an AlN adlayer at $T \sim 1800\,^\circ$C under an NH_3 atmosphere with a pressure of $P = 10^{-3}$ mbar. This termination process is followed by h-BN growth at 1600 °C to 2000 °C with NH_3 pressures ranging from 10^{-6} mbar to 10^{-1} mbar. We demonstrate epitaxial h-BN growth under unprecedented P-T conditions, characterized by

Reflection high-energy electron diffraction, Fourier transform infrared spectroscopy, Raman spectroscopy and atomic force microscopy.

DS 11.4 Wed 10:15 REC/B214

Local growth of GaAs on Si(001) and Si(001)4.5° by Laser-assisted MOVPE — •Christian Bruckmann, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institute of Physics, Otto-von-Guericke-University Magdeburg, Germany

The demand for increasingly performant, energy-efficient semiconductor devices is driving the research on how to combine III/V- with Si-based components in the most efficient way possible. While the monolithic integration on the Si substrate offers advantages compared to hybrid integration schemes, the heteroepitaxy of III/V-compound semiconductors is challenging due to different material properties. The Laser-assisted MOVPE enables an additive fabrication of semiconductor devices allowing cost-efficient low-volume production of special device structures. Key part is a high-power laser diode used for local heating of the substrate surface leading to local growth. GaAs islands were grown on Si(100) as well as Si(100) 4.5 ° substrates using a two-step growth approach which consists of a low-temperature nucleation layer followed by a high-temperature buffer layer. Optimization of the growth parameters and characterization with AFM and XRD shows qualitative trends similar to conventional MOVPE. For an island with a diameter of 260 nm and a height of 230 nm a XRD FWHM of 0.47 ° (ω-Scan, GaAs(004)) was obtained. Increasing the layer thickness to 3 μm yields a FWHM of 0.26 ° at optimum. Roughness measurements in the island center lead to RMS values of 4.0 nm (5 x 5 μm^2).

15 min. break

DS 11.5 Wed 10:45 REC/B214

Interface formation in ALD-based SnO_2/CeO_x heterostructures — •Dominic Guttmann[1], Rudi Tschammer[1], Carlos Morales[1], Malgorzata Kot[2], Michal Mazur[2], Damian Wojcieszak[2], Paulina Kapuscik[2], Wiktoria Kolodzinska[2], Jarosław Domaradzki[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus 03046, Germany — [2]Faculty of Electronics, Photonics and Microsystems, WUST, 50-372 Wroclaw, Poland

The electrical resistance of SnO_2 ultrathin films (< 20 nm) made by atomic layer deposition (ALD) strongly depends on thickness, due to intrinsic film defects at interfaces arising from changes in the ALD reaction mechanism during the first cycles and from the film/substrate interaction. Modifying interface properties in SnO_2/CeO_x heterostructures can enhance H_2 sensing performance. We studied the initial growth of SnO_2 by ALD on CeO_x substrates prepared by either electron beam evaporation (EBE) or ALD. Employing the commercial precursor tetrakis(dimethylamino)tin (TDMASn) and ozone (O_3) as well as in vacuo and near-ambient-pressure X-ray photoelectron spectroscopy, we examined how substrate preparation affects the SnO_2 nucleation behavior in the first cycles. SnO_2 growth on EBE-CeO_x indeed starts with the first precursor cycle, whereas ALD-CeO_x requires an additional conditioning step. Connecting these findings to surface chemistry, distinct C1s and N1s signatures attributed to TDMASn adsorption indicate a slow C/N buildup, consistent with previous reports on ALD-grown SnO_2 on Si, SiO_2, and Al_2O_3.

DS 11.6 Wed 11:00 REC/B214

Enhancing the antiferroelectric response of $AgNbO_3$ thin films — •Sreelakshmi Prasanna, Juliette Cardoletti, Philipp Komissinskiy, Thorsten Schneider, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Dielectric capacitors are widely utilized in numerous advanced high power electronic systems due to their distinctive features of high-power density, ultrafast charge/discharge capability, long storage lifetime, etc. Among them, antiferroelectrics have attracted extensive attention for energy storage applications because of their double hysteresis loop and zero remnant polarization. Within this class of materials $AgNbO_3$-based lead-free perovskites are promising candidates due to their environmentally friendly nature and strong intrinsic antiferroelectric response. In this work, we have grown $AgNbO_3$ thin films using pulsed laser deposition and examined their structural properties using X-ray diffraction and SEM. The presence of metallic Ag particles on the $AgNbO_3$ surface with a size ranging from nanometres to micrometres indicates excessive Ag creating conductive pathways and severely compromise the electrical performance, suppressing the antiferroelectric behaviour. We demonstrate a post-annealing and post-deposition treatment to remove excessive Ag in grain boundaries and as well as on the surface, while preserving the $AgNbO_3$ phase.This procedure reduces the leakage current significantly and enables the access to the antiferroelectric properties of $AgNbO_3$. This simple and effective way to enhance the performance of $AgNbO_3$ thin films opens the way to their application in eco-friendly energy storage devices.

DS 11.7 Wed 11:15 REC/B214

Low-Temperature Atomic Layer Deposition of Rutile Titanium Dioxide Buffer Layers for Thermochromic Windows — •Jan Leithäuser, Waafa Al Nachwati, Philip Klement, Sangam Chatterjee, and Martin Becker — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Vanadium dioxide (VO_2) exhibits a reversible semiconductor-metal transition (SMT) at approx. 68°C and enables thermochromic smart windows that modulate solar heat gain. To achieve high solar modulation (T_{sol}) at industrially compatible temperatures, a smooth, chemically stable rutile TiO_2 buffer layer is required. Here, we demonstrate that atomic layer deposition (ALD) of TiO_2 at 200 °C, followed by low-temperature annealing, results in dominant rutile at 220 °C, provided the TiO_2 thickness is at leat 30 nm; thinner layers (10 nm) crystallize as anatase. Integrating such ALD-grown rutile buffers into VO_2 || TiO_2 || Glass structures allow for optimal VO_2 growth windows at 400 - 450 °C and yields a T_{sol} comparable to that of high-temperature sputtered rutile buffers. The ALD approach maintains nanometer-scale roughness. This low-temperature route to rutile TiO_2 represents an advancement for scalable, energy-efficient thermochromic coatings compatible with temperature-sensitive substrates.

DS 11.8 Wed 11:30 REC/B214

Interface induced ferromagnetism and Superconductivity in epitaxially engineered thin films — •Mostafa Marzouk[1,2], Anupam Singh[2], Igor Mazinchenko[2], Malli Tangi[2], Sergey Ostanin[2], Younghyuk Kim[2], Ilya Kostanovski[2], Arthur Ernst[2], Mathew Gilbert[2], and Stuart Parkin[2] — [1]Current Address: Institute for Topological Insulators, University of Wuerzburg, 97074 Würzburg, Germany — [2]Max-Planck institute of Microstructure Physics, 06120 Halle (Saale), Germany

Two-dimensional electron gases (2DEGs) at oxide interfaces offer several advantages that are not typically found in semiconductor-based 2DEGs. One key advantage is their high sheet carrier density, which is essential for achieving the high current densities required in power and memory applications.

In this talk, I will present the emergent phenomena at oxide interfaces we grew using state-of-the-art molecular beam epitaxy (MBE), with a primary focus on the two-dimensional electron gases formed at KTaO-based interfaces. We observe the development of ferromagnetism in the KTaO3(110)/LaTiO3 and KTaO3(111)/LaTiO3 2DEGs. Remarkably, these ferromagnetic 2DEGs retain high electron mobilities, reaching approximately 250 cm2/V.s at 2 K and 20 cm2/V.s at 300 K. The presence of ferromagnetism is confirmed through anomalous Hall effect hysteresis loops, butterfly-shaped magnetoresistance hysteresis loops (down to 1.7 K), out-of-plane magnetization hysteresis loops, and x-ray magnetic circular dichroism (XMCD) measurements at 2 K.

DS 12: 2D Materials I

Time: Wednesday 9:30–12:00 Location: REC/C213

DS 12.1 Wed 9:30 REC/C213

Purcell enhancement of photocurrent in a van der Waals self-cavity — •Xinyu Li — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

We report the observation of Purcell-enhanced terahertz (THz) photocurrent emission in exfoliated flakes of the van der Waals (vdW) semimetal WTe_2, which act as intrinsic plasmonic self-cavities. Unlike conventional cavities that require external mirrors, micron-scale vdW flakes confine electromagnetic fields via edge reflections, supporting standing-wave plasmonic modes in the THz range. Using ultrafast optoelectronic circuitry, we measured coherent near-field THz emission resulting from nonlinear directional photocurrents excited at crystal edges. Emission spectra reveal resonant enhancement at discrete frequencies, tunable by excitation fluence and device geometry. We attribute this effect to cavity-modified photonic density of states - i.e., the Purcell effect - acting on driven, nonlinear transport currents. An analytical model capturing the self-cavity resonance conditions accurately reproduces experimental trends across multiple devices. Our findings establish WTe_2 as a bias-free, geometry-tunable THz emitter and demonstrate the potential of self-cavity engineering for controlling nonlinear, nonequilibrium dynamics in quantum materials.

Further details are available at arXiv:2507.07987.

DS 12.2 Wed 9:45 REC/C213

Radial Rashba spin-orbit fields in commensurate twisted transition-metal dichalcogenide bilayers — •Thomas Naimer[1], Paulo E. Faria Junior[2], Klaus Zollner[1], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Central Florida, Orlando, Florida 32816, USA

In commensurate twisted homobilayers, purely radial Rashba spin-orbit fields can emerge. We employ first-principles calculations to investigate the band structures and the spin-orbit fields close to the high-symmetry points K and Γ of several commensurate twisted transition-metal dichalcogenide homobilayers: WSe_2, $NbSe_2$, and WTe_2. The observed in-plane spin textures can for the most part be reproduced successfully using a model Hamiltonian, enabling us to extract relevant parameters. Exploring different lateral displacements between the layers, we confirm that the relevant symmetry protecting the radial Rashba is an in-plane 180° rotation axis. Our calculations on WTe_2 bilayers show that their lack of C_3 symmetry results in spin textures that are neither radial nor tangential. All authors acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH, the European Union Graphene Flagship project 2DSPIN-TECH (grant agreement No. 101135853) and SFB 1277 (Project-ID 314695032).

DS 12.3 Wed 10:00 REC/C213

Spatially Controlled Photoelectrochemical Thinning of 2D Transition Metal Dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Sergej Levashov[1], Franz Gröbmeyer[2], Johanna Eichhorn[1], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Technical University of Munich — [2]Ludwig Maximilian University of Munich — [3]U.S. Naval Research Laboratory

The integration of two-dimensional transition metal dichalcogenides (TMDs) into functional devices and catalytic systems requires detailed understanding and control of their behavior in reactive environments. Here, we systematically investigate the photoelectrochemical (PEC) stabilities of MoS_2, WS_2, $MoSe_2$, and WSe_2 mono- and multilayer flakes under dark and illuminated conditions, revealing two distinct oxidation mechanisms. In the dark, anodic potentials promote oxidation at defect-rich TMD edge sites, with subsequent dissolution of the oxidized species causing progressive lateral shrinkage, while the basal planes remain stable. Under white light illumination from a solar simulator, photoexcited holes drive electrochemical thinning of TMD multilayer flakes, which proceeds at anodic potentials lower than those required for lateral edge oxidation in the dark. This PEC-driven thinning enables controllable top-down fabrication of large-area TMD films with well-defined thicknesses. Importantly, the use of a focused laser beam rather than white light illumination enables precise spatial control over the PEC oxidation process, allowing localized patterning and thinning in predefined regions for the processing and integration of 2D materials into functional devices.

DS 12.4 Wed 10:15 REC/C213

Pairing symmetry of Ising superconductors via the upper critical field — •Lena Engström[1], Ludovica Zullo[2], Tristan Cren[3], Andrej Mesaros[1], and Pascal Simon[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France

Several conflicting predictions have been made for the symmetry of the pairing in transition metal dichalcogenide (TMD) superconductors. An indication of if singlet or triplet pairing is present can be given by the upper critical field (Hc2), the magnetic field required to fully suppress superconductivity. Monolayer 1H-NbSe2 and 1H-TaS2 have extremely large critical fields, due to a large Ising spin-orbit coupling (SOC), yet they do not scale with SOC and temperature as expected for other TMDs. In our work on few-layer 2H-stacked TMDs, we highlight that the Ising SOC has nodal lines in the Brillouin zone imposed by symmetry. By deriving the susceptibility, we have found that the scaling of the critical field can be traced back to whether the Fermi surface intersects with these lines or not. Reinterpreting existing experimental data, we find that a predominantly singlet order is consistent with the measured Hc2. We propose two experiments where a signature of spin-singlet pairing would be visible, while discussing the possibility of mixed-parity pairing.

DS 12.5 Wed 10:30 REC/C213

Single-Metal-Atom Chains in Transition-Metal Dichalcogenides: Electronic, Magnetic, and Catalytic Properties — •Prosun Santra, Mahdi Ghorbani-Asl, and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

One-dimensional metallic nanostructures exhibit Peierls instabilities, Tomonaga-Luttinger liquid behavior, Majorana fermions, and half-metallicity, which is interesting in the context of spintronics. Stable single-metal-atom chains (SMACs) were experimentally manufactured by embedding transition metal (TM) atoms at mirror twin boundaries (MTBs) in MoS_2. Using DFT calculations, we study the energetics and properties of SMACs formed by 21 TM elements embedded in MTBs in 2D $MoSe_2$, $MoTe_2$, WS_2, and WSe_2. Spin-polarized calculations reveal localized magnetism and half-metallicity in multiple systems, ideal for nanoscale spintronics. We further study the catalytic properties of these systems. Our results indicate that selected SMACs can surpass Pt(111) in hydrogen evolution reaction activity, so that these defect-engineered structures not only are versatile 1D quantum-spintronic platforms, but may also be utilized as low-cost, high-performance electrocatalysts for green H_2 production.

15 min. break

DS 12.6 Wed 11:00 REC/C213

Magnetoelectric flat band induced by a $\sqrt{3} \times \sqrt{3}$ charge density wave in monolayer $CrSe_2$ — •Victor Pardo[1], Pablo Savino Real[1], Carmen Fuente Santiago[1], Jan Phillips[2], Javier Corral Sertal[1], Adolfo Otero Fumega[3], and Santiago Blanco Canosa[4] — [1]Instituto de Materiais iMATUS, Universidade de Santiago de Compostela, E-15782 Campus Sur s/n, Santiago de Compostela, Spain — [2]Iberian International Nanotechnology Laboratory, INL Braga, Portugal — [3]Department of Applied Physics, Aalto University, 02150 Espoo, Finland — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

We investigate the electronic and magnetic properties of the $\sqrt{3} \times \sqrt{3}$ charge-density-wave (CDW) phase of $CrSe_2$ using first-principles calculations within density functional theory. We find that the most stable configuration corresponds to a ferromagnetic ground state, which hosts a remarkably flat electronic band exactly at the Fermi level. We show that the flat band derives from an a_{1g}-like component of the Cr t_{2g} manifold in a trigonal environment, combined with bonding–antibonding splittings induced by the formation of Cr trimers in the CDW structure. Strong hybridization between Cr d and Se p orbitals is

crucial for stabilizing this band exactly at the Fermi level. Spin–orbit coupling affects only the remaining d bands, leaving the flat band intact. We establish how to tune the existence of this flat-band by relating it to the electric polarization caused by the CDW, hence describing a mechanism to turn on/off strong correlations with an external tuning parameter such as an electric field.

DS 12.7 Wed 11:15 REC/C213

Topological Superconductivity in $NbSe_2$-based Ising-Type Superconductors — •Jozef Haniš[1], Marko Milivojević[2], Zoltan Tajkov[3], and Martin Gmitra[1] — [1]Institute of Experimental Physics SAS Watsonova 47 040 01 Košice, Slovak Republic — [2]Institute of Informatics, Slovak Academy of Sciences, Dúbravská cesta 9 845 07 Bratislava 45, Slovakia — [3]Eötvös Loránd University, Pázmány Péter sétány 1/A, Budapest, Hungary

Topological superconductivity offers the promise of Majorana-bound states for fault-tolerant computation. We develop a symmetry-guided framework for superconducting pairing in Ising-type transition metal dichalcogenides, focusing on $NbSe_2$-based systems. We identify multiple topological phases–classified by Chern numbers and $\mathbb{Z}_2$ invariants–enabled by spin-orbit-induced triplet pairing. We present topological phase diagrams for different doping regimes and discuss zigzag-ribbon band-structure calculations. This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00071, and the Slovak Academy of Sciences project IMPULZ IM-2021-42.

DS 12.8 Wed 11:30 REC/C213

Modeling Pressure-Induced Exciton Screening in hBN/WSe2/hBN Heterostructures — •Adlen Smiri[1], Shalini Badola[2], Amit Pawbake[2], Clément Faugéras[2], and Iann C. Gerber[1] — [1]Université Fédérale de Toulouse Midi Pyrénées, INSA-CNRS-UPS, LPCNO, 135 Av. de Rangueil, 31077 Toulouse, France — [2]Laboratoire National des Champs Magnétiques Intenses, LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSA-T, Grenoble and Toulouse, France.

Hydrostatic pressure is an effective tool to tune excitonic properties in two-dimensional semiconductors. We investigate the pressure dependence of excitonic Rydberg states in a WSe2 monolayer encapsulated in hBN and observe a reduction of the 1s-2s and 1s-3s energy separations with increasing pressure. First-principles calculations indicate negligible changes in the band structure and effective masses, pointing to pressure-modified dielectric screening as the main mechanism. A microscopic dielectric model for the WSe2 monolayer with an effective vacuum gap reproduces the observed excitonic shifts, demonstrating that enhanced screening governs exciton renormalization. These results provide a quantitative framework for tuning excitonic interactions in van der Waals heterostructures.

DS 12.9 Wed 11:45 REC/C213

Above room temperature ferromagnetism in wafer-scale Fe_3GaTe_2/SiC and the origin of double-step hysteresis in MBE-grown Fe_3GaTe_2 films — •Tauqir Shinwari[1], Victor Ukleev[2], Chen Luo[2], Kacho Imtiyaz Ali Khan[1], Florin Radu[2], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz Zentrum Berlin for Materialien und Energie, Albert-Einstein Straße 15, 12489 Berlin, Germany

Two-dimensional (2D) magnetic materials provide a versatile platform for next-generation spintronic devices, where scalable growth and robust ferromagnetism are the key factors. Fe_3GaTe_2 is a 2D ferromagnet with a high Curie temperature ($\sim$ 360K) and strong perpendicular magnetic anisotropy, making it a particularly promising candidate for energy-efficient spin-based technologies. Until now, most studies on Fe_3GaTe_2 have relied on millimeter-sized bulk crystals and exfoliated flakes, which are unsuitable for wafer-scale integration and reproducible device processing. In this work, we demonstrate high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films directly on SiC(0001) substrates by MBE. The films exhibit robust above-room-temperature ferromagnetism together with strong out-of-plane magnetic anisotropy, as confirmed by magnetometry and element-specific x-ray techniques. A double-step hysteresis loop is observed in MBE-grown Fe_3GaTe_2 films, pointing to the coexistence or coupling of distinct magnetic subsystems, which will be discussed in the context of Fe site selectivity, thickness dependence, and interfacial effects.

DS 13: Layer Properties

Time: Wednesday 15:00–16:15 Location: REC/B214

Invited Talk DS 13.1 Wed 15:00 REC/B214

Tailored thermal treatments for multi-layer, multi-material polymer devices — •Katherina Haase, Shaoling Bai, Mike Hambsch, Vojtech Millek, and Stefan C. B. Mannsfeld — Faculty of Electrical and Computer Engineering & Center for Advancing Electronics Dresden (cfaed), TUD Dresden University of Technology, 01069 Dresden, Germany

Thermal annealing constitutes an important processing step during the fabrication of organic semiconductor-based devices as it removes residue solvent and often leads to improved structural order. Recently, we have explored an additional aspect of thermal annealing - its impact on the dissolution of conjugated polymer (CP) thin films. We could show that thermal annealing induces physical cross-linking in a wide range of CPs,[1] which distinctly increased their stability in the original solvent. Hence, we suggested that tailored thermal treatments could enable polymer heterojunction devices though simple sequential coating.

In this presentation, we discuss the important finding that the thermal physical cross-linking (TPC) effect produces solvent-resistant thin films for a wide variety of CPs that could be combined into a multitude of novel devices, and explore the fabrication of solution-coated, polymer heterojunction-based synaptic transistors - devices that could not have been realized without the application of cross-linking.

[1] S. Bai, K. Haase, J. Perez Andrade, M. Hambsch, F. Talnack, V. Millek, A. Prasoon, J. Liu, K. Arnhold, S. Boye, X. Feng, S. C. B. Mannsfeld, Adv. Electron. Mater. 2024, 10, 1.

DS 13.2 Wed 15:30 REC/B214

Mechanical Stress Evolution in Polycrystalline Ge Thin Films under MeV Ion Irradiation — •Karla J. Paz Corrales[1], Aaron Reupert[2], Kevin Lubig[2], Frank A. Müller[2], Berit Marx-Glowna[3], Ralf Röhlsberger[3], Till Weickhardt[1], Giancarlo Soavi[1], Martin Hafermann[1], Elke Wendler[1], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Helmholtz-Institut Jena, Fraunhoferstr. 8, 07743 Jena, Germany

Polycrystalline Ge thin films were deposited by magnetron sputtering, annealed at 600 °C for 1 h, and irradiated with 1.8 MeV Au ions over a broad fluence range. Structural, optical, and in-situ mechanical stress analyses were performed to investigate irradiation-induced property modifications. At low fluences, the films show a reduction of the initial tensile residual stress from the preparation process. This stress compensation is linked to the formation of point defects, which also decrease the optical band gap. These defects can migrate to grain boundaries, where recombination enhances the resistance to amorphization compared with single-crystalline Ge. At higher fluences, defect accumulation increases tensile stress and leads to the formation of mixed polycrystalline-amorphous phases. With further irradiation, the films fully transform into an amorphous phase, as evidenced by changes in both structural and optical properties. In this amorphous state, additional stress relaxation occurs, attributed to plastic flow or to interface effects between the film and substrate.

DS 13.3 Wed 15:45 REC/B214

Optical tuning of Sr(Mo,Ti)O_3 thin films through solid solution — •Anjima Kallam Valli, Juliette Cardoletti, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Transparent conductive oxides are key materials in display technology and renewable energy applications, being used as transparent electrodes in solar cells and optoelectronic devices. Perovskite oxides such as $SrMoO_3$, $SrVO_3$, and $SrNbO_3$ exhibit exceptional metallic conduc-

tivity combined with optical transparency. Among them, bulk $SrMoO_3$ shows a conductivity of 2 * 10^7 S m $^{-1}$ exceeding that of platinum at room temperature; however, its optical transparency is limited to the UV visible range (300 to 500 nm). This work investigates the broadening of the transparency window of $SrMoO_3$ through partial B-site substitution of molybdenum by titanium. Titanium incorporation modifies the carrier density and thereby tunes the plasma frequency, shifting the optical reflection edge toward longer wavelengths. Epitaxial Ti-substituted $SrMoO_3$ thin films have been grown by pulsed laser deposition. Structural analysis was performed by XRD, and their electrical transport properties, including resistivity and carrier density, were characterised using van der Pauw and Hall-effect measurements. Optical transparency has been evaluated by spectroscopic analysis. Through tailoring of the transparency with varying Ti concentration, this work opens the door to various optoelectronic device applications.

DS 13.4 Wed 16:00 REC/B214

Automating calculations for advancing the simulations of solid interfaces — •Elisa Damiani, Margherita Marsili, and Maria Clelia Righi — Dipartimento di Fisica e Astronomia, University of Bologna, Italy

Solid-solid interfaces are ubiquitous and simulations help understanding their properties, and may represent powerful screening and designing tools. Often first-principles electronic structure methods must be used: for example to characterize their transport, electronic, optical and magnetic properties, and also their adhesion and friction. Nevertheless, these approaches comes along with computational complexity and costs. In this talk I will present how we address these computational challenges by developing TribChem, a software that automates the creation of interface models, the identification of the optimal computational parameters, job submission, and data retrieval and storage. I will also show how this code has been successfully applied to the systematic study of different classes of interfaces such as metal-metal, metal-semiconductor, and metal-2D-materials ones, and illustrate the current developments that carried out to increase the complexity of the systems that can be addressed (amorphous and molecular solids) employing a Bayesian Optimization approaches.

These results are part of the SLIDE project that has received funding from the European Research Council (ERC) under the European Union*s Horizon 2020 research and innovation program (Grant agreement No. 865633).

DS 14: 2D Materials II (joint session DS/HL)

Time: Wednesday 15:00–17:30 Location: REC/C213

DS 14.1 Wed 15:00 REC/C213

Engineering at the Thinnest Scale: Insights into the Stability of 2D GaN on Liquid Metal Catalysts — •Tomoko Yokaichiya, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Hexagonal GaN (h-GaN), theorized to be metastable when confined to only a few nanometers, stands out as a promising wide-bandgap semiconductor for next-generation nanoelectronics. Although early studies report that h-GaN can be synthesized using e.g. liquid metal catalysts, its definitive experimental identification is challenging. This difficulty arises from a structural ambiguity due to possible defects, multilayer-stacking variations, and competing polymorphs of h-GaN's characteristic honeycomb structure, as predicted by pioneering, yet simplified electronic-structure studies. In this work, we use density functional theory alongside large-scale atomistic simulations based on machine-learned interatomic potentials to re-assess the stability of h-GaN at finite temperatures and in the presence of a liquid metal substrate. We systematically investigate the structural and electronic properties of h-GaN, examining how they evolve with layer thickness and possible structural variations. Furthermore, we analyze its thermodynamic competition with bulk wurtzite GaN and alternative thin-film polymorphs, including a previously suggested haeckelite phase. Our results reveal that h-GaN exists within a delicate stability window. Based on these insights, we propose key signatures to guide experimental detection and outline whether h-GaN may become synthesizable as a feasible 2D semiconductor.

DS 14.2 Wed 15:15 REC/C213

Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ — •Timon Mosko[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Safarik University in Kosice, Park Angelinum 9, 04001 Kosice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Kosice, Slovakia

The monolayer α-$TaSi_2N_4$ belongs to the recently discovered MA_2Z_4 family of two-dimensional intercalated materials, exhibiting wide range of physical properties, including semiconducting, metallic, topological, and superconducting behavior. Members of this group, such as $MoSi_2N_4$, WSi_2N_4 have already been successfully synthesized, highlighting the structural and electronic tunability of the inspected group of materials. We investigated the superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ using a combination of ab initio and effective model approaches. The phonon-mediated superconductivity is examined through first-principles calculations, an effective tight-binding Hamiltonian in Wannier basis and further analyzed within the Migda-Eliashberg theory of superconductivity. Our results reveal that α-$TaSi_2N_4$ is an anisotropic two-band superconductor. Additionally, we study the dielectric response via electric susceptibility using linear response theory within the RPA, combining Green's function formalism with tight-binding modeling.

This work was supported by the Slovak Academy of Sciences project IMPULZ IM-2021-42, and by the Ministry of Education, Research, Development and Youth of the Slovak Republic, provided under Grant No. VEGA 1/0104/25.

DS 14.3 Wed 15:30 REC/C213

Probing the Quantum Spin Hall State in Atomic Monolayers via NanoARPES — •Cedric Schmitt[1,2], Lukas Gehrig[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Matthew Watson[3], Jörg Schäfer[1,2], Simon Moser[1,2,4], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Diamond Light Source, UK — [4]AG Oberflächen, Ruhr-Universität Bochum

Our recently discovered quantum spin Hall insulator indenene [1], a triangular monolayer of indium on SiC(0001), exhibits a 120 meV gap and monodomain growth on the μm scale. To verify its topological nature, we use circular dichroism in ARPES as a bulk-sensitive probe of orbital angular momentum (OAM) linked to its Berry curvature [2]. Due to SiC's stepped morphology, stacking-dependent OAM cancellation complicates microARPES. We overcome this challenge using nanoARPES with sub-600 nm resolution, resolving OAM asymmetry at individual terraces of SiC. Our study establishes dichroism as a robust spectroscopic tool for topological classification within a single SiC terrace.

[1] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)
[2] J. Erhardt et al. Phys. Rev. Lett. 132, 196401 (2024)

DS 14.4 Wed 15:45 REC/C213

Physical Properties of $Ti_3C_2Cl_2$ MXenes — •Moritz Vanselow[1], Maksim Riabov[2], Thierry Ouisse[2], Hanna Pazniak[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

Hydrophobic $Ti_3C_2Cl_2$ MXenes are synthesized by Lewis acid molten-salt etching of $Ti_3C_2Cl_2$ followed by delamination process[1] and subsequently deposited from acetonitrile suspension ($\sim$ 0.1 mg/mL) on $Si(100)/SiO_2$ substrates. Using in-situ mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum, we show that $Ti_3C_2Cl_2$ exhibits enhanced thermal robustness up to 900°C as compared to conventional mixed-terminated $Ti_3C_2T_x$ MXenes with $T_x = -F, = O$, and $-OH$. Complementary ex situ XRD and XPS confirm the absence of intercalated water and uniform $-Cl$ terminations, resulting in sharp and intense (00l) peaks with $c = 2.223 \pm 0.015$ nm and reflecting its high degree of structural order. Low-temperature specific heat measurements reveal distinct phonon signatures expected for the two-dimensional $Ti_3C_2Cl_2$. We determined the Debye temperature to 548 K in a temperature interval 20–50 K consistent with DFT model calculations[2] and a Sommerfeld constant of $\gamma = 19.2\,\mathrm{mJ\,mol^{-1}\,K^{-2}}$. This work is supported by ANR-23-CE09-

0031-01 and DFG ID 530103526.

[1] T. Zhang et al., Chem. Mater. 36, 1998 (2024). [2] M. Riabov, M. Vanselow, et al., npj 2D Materials & Applications 2025, accepted

DS 14.5 Wed 16:00 REC/C213

Phase field crystal model of out-of-plane deformations in thin crystalline sheets induced by thermal expansion — •Emma Radice[1], Marco Salvalaglio[1,2], and Axel Voigt[1] — [1]Institut für Wissenschaftliches Rechnen, Technische Universität Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Thin, flexible crystalline sheets exhibit unique elastic properties due to their ability to undergo out-of-plane deformations.Understanding this behavior requires a description that couples in-plane elasticity, out-of-plane bending and the presence of defects. We develop a mesoscale description for these systems by extending the Phase-Field Crystal (PFC) model. PFC model describes crystal structures at diffusive timescales through a periodic, microscopic density field and it allows one to incorporate both elasticity and topological defects into a continuum description. Our extension permits a spatially varying equilibrium lattice spacing, enabling the representation of localized lattice eigenstrain to mimick thermal effects or lattice mismatch in heterostructures. We validate the extended model against analytical predictions from the Föppl von Kármán equations for uniaxial compression and from Eshelby's inclusion problem. Using this validated framework, we then study how locally induced compressive stresses drive out-of-plane deformation (buckling) in the sheets. Our approach, implemented via a Fourier pseudo-spectral method, exploits the PFC model's natural ability to capture the complex, coupled interactions among elasticity, out-of-plane bending and defect dynamics.

15 min. break

DS 14.6 Wed 16:30 REC/C213

Magnetotransport in Z-Folded ABC-Stacked Trilayer Graphene Structures — •Maximilian Mischke, Lina Bockhorn, Sofiya Lazareva, and Rolf Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Folded graphene (multi)layers promise to contain rich and interesting physics [1-3], so we produced a sample to investigate the influence of such a fold on magnetotransport properties of graphene. The measurements were carried out in a 4He cryostate at 1.4 K while the samples' carrier concentration was controlled via a global backgate. The sample itself consists of a z-folded ABC-trilayer graphene partially encapsulated in hBN with electrical contacts that allow for measurements in the unfolded region as well as through the fold. We observed filling factors that are unexpected for ABC-trilayer graphene. The untypical transport behaviour can be explained by angle dependend interlayer coupling and screening effects in the z-fold.

[1] S. J. Hong et al, Phys Rev B 105, 205404 (2022)
[2] H. Schmidt et al, Nature Communications 5(1), 5742 (2014)
[3] Y. Liu et al, Phys Rev B 92, 235438 (2015)

DS 14.7 Wed 16:45 REC/C213

Quantum dots in proximitized BLG/TMD heterostructures — •Ching-Hung Chiu and Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

Bilayer graphene (BLG) has attracted attention recently due to the possibility of inducing layer-selective Spin-orbit coupling (SOC) by proximitizing with transition metal dichalcogenides (TMDs) [1,2]. Simultaneously, the gate-tunable band gap in BLG enables electrostatic confinement of charge carriers into gate-defined quantum point contacts and quantum dots [3,4]. Here, we theoretically investigate the interplay of proximity effects and confinement by studying confined quantum states in proximitized BLG/TMD quantum dots. We calculate the states' properties, such as their splittings and spin polarisation, as a function of SOC coupling parameters and the dot's size and shape. Our studies go alongside experimental realisations of confinement in BLG/TMD heterostructures [5,6] and pave the way for using and controlling the dot's spin and valley states as qubits.

[1] K. Zollner and J. Fabian, Phys. Rev. B 104, 075126 (2021)
[2] A. M. Seiler et al., 2025 2D Mater. 12 035009
[3] H. Overweg et al,, Phys. Rev. Lett. 121, 257702 (2018)
[4] S. Möller et al., Phys. Rev. Lett. 127, 256802 (2021)
[5] J. D. Gerber et al., Nano Lett. 2025, 25, 33, 12480-12486
[6] H. Dulisch et al., Nano Lett. 2025, 25, 26, 10549-10555

DS 14.8 Wed 17:00 REC/C213

Influence of Polymethyl Methacrylate molecular weight on Graphene transfer and its intrinsic properties — •Monika Choudhary[1], Rasuole Lukose[1], Moriom Akter[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]Leibniz-Institut für Innovative Mikroelektronik (IHP), Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

Polymethyl methacrylate (PMMA)-assisted wet transfer is widely used for integrating large-scale graphene grown on Ge(100)/Si substrates via chemical vapor deposition onto insulating SiO2/Si substrates[1,2]. However, the influence of PMMA molecular weight (MW) on properties of transferred graphene is insufficiently quantified. To address this, we investigate graphene transferred using low (50K), medium (600K), and high (950K) MW PMMA to isolate how polymer chain length governs film integrity and contamination. Characterization by atomic force microscopy (AFM), and spatially resolved X-ray photoelectron spectroscopy (XPS) reveals reduced contamination and smoother topography for graphene with 600K transfers. Additionally, micro-Raman spectroscopy demonstrates strain-free graphene with reduced doping and a 2D peak full width at half maximum (FWHM) of 35.53 cm-1 consistent with as-grown values. 1. Akhtar F., et al. ACS Appl. Mater. Interfaces 15 (2023). 2. Lukose R., et al. Scientific Reports 11 (2021). Acknowledgement: This research was funded by the European Union*s Horizon Europe research and innovation programme under grant agreement No 101120938 (GATEPOST).

DS 14.9 Wed 17:15 REC/C213

High-performance graphene field-effect transistors on cyclic olefin copolymer substrates for advanced sensor applications — •Hamid Reza Rasouli[1], Begimai Adilbekova[1], Ghazaleh Eshaghi[1], Axel Printschler[1], David Kaiser[1], Marco Reinhard[2], Alexander Rolapp[2], Tom Reinhold[2], Uwe Hübner[3], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]IMMS Institut für Mikroelektronik- und Mechatronik-Systeme gemeinnützige GmbH (IMMS GmbH), 99099 Erfurt, Germany — [3]Leibniz Institute of Photonic Technology, Albert-Einstein-Straße 9, 07745 Jena, Germany

While graphene field-effect transistors (GFETs) are highly attractive for liquid-phase sensing, their performance on SiO2/Si substrates is compromised by oxide-induced charge trapping, leading to pronounced hysteresis and reduced stability. We present arrays of GFETs microfabricated on cyclic olefin copolymer (COC) substrates, which passivate SiO2 providing a low-trap and chemically inert platform in combination with flatness. GFET devices on COC demonstrate remarkably improved Dirac point stability, negligible hysteresis even in low-ionic strength buffers, and reproducibility across the arrays. For their functionalization, we employ an ultrathin carbon nanomembrane (CNM) that enables robust immobilization of various capture molecules while preserving graphene's transport properties. The CNM/GFET/COC architecture provides stable liquid-phase operation highlighting its strong potential for scalable and advanced sensor applications.

DS 15: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)

Time: Thursday 9:30–12:30 Location: HSZ/0003

DS 15.1 Thu 9:30 HSZ/0003

Bulk High-Temperature Superconductivity and Density Waves in Layered Nickelates — •Jun Luo[1,2], Jie Dou[1,2], Shuo Li[1], Qin Xin Shen[1,2], Xu Yang Feng[1,2], De Min Chai[1,2], Ran Sheng Jia[1,2], Jie Yang[1,2], and Rui Zhou[1,2] — [1]Institute of Physics, Chinese Academy of Sciences, and Beijing National Laboratory for Condensed Matter Physics, Beijing 100190, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

The recent advances in bilayer nickelates $La_3Ni_2O_7$ have revealed fascinating high-temperature superconductivity (HTSC) under high-pressure conditions, offering a promising platform to explore unconventional superconducting mechanisms. In this talk, I will first discuss the discovery of bulk HTSC in Pr-doped $La_2PrNi_2O_7$, where Pr substitution effectively suppresses intergrowth phases, resulting in nearly pure bilayer structures. Superconducting onset temperature reaches 82.5 K at 16 GPa. Clear diamagnetic signals confirm the bulk nature of HTSC. I will also present microscopic evidence of charge and spin density wave (CDW/SDW) orders in $La_3Ni_2O_7$, revealed through 139La nuclear quadrupole resonance (NQR). Below the density wave transition temperature, we observe distinct line splitting and magnetic broadening, indicating unidirectional CDW order coupled with SDW order. By integrating insights from high-pressure and NQR studies, this work provides a comprehensive understanding of the structural and electronic mechanisms underlying HTSC in bilayer nickelates, paving the way for future experimental and theoretical investigations.

DS 15.2 Thu 9:45 HSZ/0003

ARPES spectra and the role of interstitial-*s* orbital in infinite-layer nickelates calculated by DFT+DMFT — •Leonard Verhoff[1], Liang Si[1,2], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Wien, Austria — [2]School of Physics, Northwest University, Xi'an, China

Infinite-layer nickelates, such as $NdNiO_2$, are a compelling platform to explore the microscopic origin of unconventional high-temperature superconductivity, from both theoretical and experimental perspectives.

Experimentally, infinite-layer nickelates are reduced from the stable perovskite phase, leaving an empty apical oxygen site. *Density functional theory* (DFT) calculations show that the resulting interstitial vacancy hosts localized, *s*-like states about 2 eV above the fermi level, while recent *angle-resolved photoemission spectroscopy* (ARPES) measurements of superconducting $NdNiO_2$ thin films conjectured Fermi surfaces with major *s*-like orbital character, highlighting a possible role of interstitial-*s* states in superconductivity.

We present DFT and *dynamical mean field theory* calculations of Fermi surfaces and band structures for both bulk and slab geometries, directly comparable to ARPES spectra. Our ARPES simulations explicitly include first-principles photoemission matrix elements, capturing the impact of orbital shapes on the measured intensity. We show how the correlated band structure reproduces low-energy ARPES spectra and identify the features dominated by interstitial-*s* character.

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; FWF project ID I5398.

DS 15.3 Thu 10:00 HSZ/0003

A photoinduced two-dimensional electron gas (2DEG) at infinite-layer nickelate/strontium titanate interfaces — •D. Sanchez-Manzano[1], G. Krieger[2], A. Raji[3], B. Geisler[4], V. Humbert[1], H. Jaffres[1], J. Santamaria[5], R. Pentcheva[4], A. Glotter[3], D. Preziosi[2], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, France. — [2]Institute of Physics and Chemistry of Materials of Strasbourg, CNRS, University of Strasbourg, France. — [3]Laboratoire de Physique de Solides, CNRS, Université Paris-Saclay, France. — [4]Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [5]6Departamento de Física de Materiales, Universidad Complutense de Madrid, Spain

We demonstrate, through experiments (transport, electron microscopy & spectroscopy) and density functional theory (DFT), that a high-mobility 2DEG can be optically switched on and off at an oxide interface where such a state does not naturally exist [1]. We show that near-ultraviolet light instantly creates a volatile 2DEG at the interface between $SrTiO_3$ (a band insulator) and infinite-layer $NdNiO_2$ (a poor metal), resulting in a conductivity increase of up to five orders of magnitude. This stems from structural and electronic reconstructions that, along with a built-in interfacial electric field, facilitate the Ti-3d band occupation by photogenerated carriers. These findings open venues for engineering photoconductance in strongly correlated systems.

[1] Sanchez-Manzano et al., Nat. Mater. (2025). https://doi.org/10.1038/s41563-025-02363-y

DS 15.4 Thu 10:15 HSZ/0003

Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition — •Lucía Iglesias[1], Dongxin Zhang[1], Aravind Raji[2,3], Luis M. Vicente-Arche[1], Alexandre Gloter[2], and Manuel Bibes[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay — [3]Synchrotron SOLEIL

Superconductivity in infinite-layer (IL) nickelates (ABO_2) was discovery in 2019, opening a new research frontier. However, progress remains limited by the challenging topotactic reduction needed to remove all apical oxygens from the perovskite precursor, typically achieved through a complex ex situ CaH_2 method. Although recent in situ approaches, such as metal overlayer deposition via molecular beam epitaxy and atomic hydrogen bombardment, have improved control and reproducibility, their restricted accessibility highlights the need for simpler synthesis routes. Here, we demonstrate a broadly accessible method to fabricate superconducting IL $Pr_{0.8}Sr_{0.2}NiO_2$ films via aluminum deposition using direct-current magnetron sputtering. The sputtered Al drives the reduction through a redox reaction, converting the precursor perovskite into the superconducting IL phase. Systematic optimization of Al-induced reduction yields high-quality films with a maximum transition temperatures of 17 K, consistent with the best reported values. This accessible and highly reproducible approach provides an effective alternative to existing techniques and lowers barriers to the exploration of nickelate superconductors.

DS 15.5 Thu 10:30 HSZ/0003

Two-dimensional vortex matter in infinite-layer nickelates — •David Sanchez-Manzano[1], Vincent Humbert[1], Araceli Gutiérrez-Llorente[1,2], Dongxin Zhang[1], Jacobo Santamaría[3], Manuel Bibes[1], Lucia Iglesias[1], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Univerisité Paris-Saclay, 91767 Palaiseau, France — [2]Escuela Superior de Ciencias Experimentales y Tecnología, Universidad Rey Juan Carlos, 28933 Madrid, Spain — [3]GFMC, Dpto. de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

Characterizing the dimensionality of the superconducting state in the infinite-layer (IL) nickelates is crucial to understanding its nature. Most studies have addressed the problem by studying the anisotropy of the upper critical fields. Yet, the dominance of Pauli-paramagnetism effects over orbital ones makes it challenging to interpret the experiments in terms of dimensionality. Here we address the question from a different perspective, by investigating the vortex phase diagram in the mixed-state. We demonstrate that superconducting $Pr_{0.8}Sr_{0.2}NiO_2$ thin films present a vortex liquid-to-glass transition of a two-dimensional nature. The obtained results suggest that bidimensionality is an intrinsic property, and that superconductivity resides in fully-decoupled NiO_2 planes. In this scenario, the coherence length along the c-axis must be shorter than the distance between those planes, while Josephson and magnetostatic coupling between them must be negligible. We believe that these conclusions are relevant for theories on the origin of superconductivity in the IL-nickelates.

DS 15.6 Thu 10:45 HSZ/0003

Systematically Controlled Disorder to Probe Pairing Symmetry in Infinite-Layer Nickelates — •A. Ranna[1], R. Grasset[2], M. Gonzalez[3], K. Lee[3], B. Y. Wang[3], D. Zhang[4], W. Sun[5], C. Parzyck[6], Y. Wu[6], M. Konczykowski[2], M. Bibes[4], K. M. Shen[6], Y. F. Nie[5], L. Iglesias[4], H. Y. Hwang[3], A. P. Mackenzie[1], and B. H. Goodge[1] — [1]MPI CPfS, Germany — [2]LSI, Ecole Polytech-

nique, France — [3]Stanford University, USA — [4]CNRS Thales, France — [5]Nanjing University, China — [6]Cornell University, USA

Superconductivity in infinite-layer nickelates has expanded rapidly with advances in thin-film synthesis and reduction techniques. A central question is the symmetry of the superconducting gap in these materials. Because superconducting samples can only be stabilized as thin films and suffer surface degradation during the post-growth reduction process, some conventional probes to determine the gap symmetry remain challenging to perform and interpret. Here, we leverage high-energy electron irradiation to controllably introduce point-like defects without altering film stoichiometry or crystallinity. Tracking superconductivity with systematically increasing disorder shows a steady suppression of transition temperature and rising normal state resistivity, indicative of an unconventional, sign-changing gap [1] . Additionally, this method offers a unique way to study the effect of point defects on superconducting and electronic properties in nickelates across rare-earth compositions, doping, and strain to disentangle intrinsic behavior from synthesis-related variability.

[1] Ranna et al., *PRL* **135**, 126501 (2025).

15 min. break

DS 15.7 Thu 11:15 HSZ/0003

Correlated electronic structure of $La_3Ni_2O_6$ and $La_3Ni_2O_{6.5}$ — •Frank Lechermann, Steffen Bötzel, and Ilya M. Eremin — Theoretische Physik III, Fakultät für Physik und Astronomie, Ruhr-Universität Bochum, Bochum, Germany

There are two known superconducting nickelate families, i.e. low-valence Ni($3d^{9-\delta}$) compounds and Ruddelsden-Popper (RP) compounds with Ni($3d^{8\pm\delta}$) valence. While both families host NiO_2 square planes, key difference is given by the missing apical oxygen atoms in the low-valence nickelates. A possible route to connect both nickelate families might be given by the reduction of the $La_3Ni_2O_7$ RP bilayer compound, i.e. by removing it's apical oxygens. Complete removal results in the $La_3Ni_2O_6$ compound, while taking out only half of the apical oxygens results in the $La_3Ni_2O_{6.5}$ compound. Both reduced materials are so far only scarcely characterized experimentally, but display quite intriguing correlation physics from theory. We will discuss the results of advanced first-principles many body calculations for these two nickelates, highlighting different mechanisms of Mott criticality as well as challenging low-temperature physics.

DS 15.8 Thu 11:30 HSZ/0003

Superconductivity governed by Janus-faced fermiology in strained bilayer nickelates — •Siheon Ryee[1], Niklas Witt[2], Giorgio Sangiovanni[2], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany

High-temperature superconductivity in pressurized and strained bilayer nickelates has emerged as a new frontier. One of the key unresolved issues concerns the fermiology that underlies superconductivity. On both theoretical and experimental sides, no general consensus has been reached, and conflicting results exist regarding whether the relevant Fermi surface involves a γ pocket—a hole pocket with d_{z^2}-orbital character centered at the Brillouin zone corner. Here, we address this issue by unveiling a Janus-faced role of the γ pocket in spin-fluctuation-mediated superconductivity. We show that this pocket simultaneously induces dominant pair-breaking and pair-forming channels for the leading $s_\pm$-wave pairing. Consequently, an optimal superconducting transition temperature T_c is achieved when the γ pocket surfaces at the Fermi level, placing the system near a Lifshitz transition. This suggests that superconductivity can emerge, provided the maximum energy level of the γ pocket lies sufficiently close to the Fermi level, either from below or above. Our finding not only reconciles two opposing viewpoints on the fermiology, but also naturally explains recent experiments on $(La,Pr)_3Ni_2O_7$ thin films, including the superconductivity under compressive strain, two conflicting measurements on the Fermi surface, and the dome shape of T_c as a function of hole doping.

DS 15.9 Thu 11:45 HSZ/0003

Bonding-antibonding $s_\pm$ superconductivity in bilayer nickelates: potential experimental signatures — •Steffen Bötzel, Frank Lechermann, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Germnay

The discovery of high-T_c superconductivity in Ruddelsden-Popper bilayer nickelates under applied high pressure and/or compressive strain provides a promising platform to study the interplay of multiorbital intralayer and interlayer Cooper-pairing in bilayer systems. In particular, dominant interlayer pairing may naturally lead to a bonding-antibonding $s_\pm$-gap structure, which directly reflects the bilayer geometry. Such a scenario would produce characteristic experimental signatures that differ from d-wave type gap symmetries. In this contribution, we theoretically address the possible gap structures in bilayer nickelates and discuss how a interlayer-dominated bonding-antibonding $s_\pm$-gap structure can be potentially distinguished from a d-wave type pairing using experimentally observables.

DS 15.10 Thu 12:00 HSZ/0003

Interlayer interaction-driven $s^\pm$-to-d_{xy}-wave superconductivity in $La_3Ni_2O_7$ under pressure — •Lauro B. Braz[1], George B. Martins[2], and Luis G. G. de V. D. Da Silva[1] — [1]Instituto de Física, Universidade de São Paulo, Rua do Matão 1371, São Paulo, São Paulo 05508-090, Brazil — [2]Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Minas Gerais 38400-902, Brazil

Experimental and theoretical progress on the normal-state properties of the high-temperature superconductor $La_3Ni_2O_7$ has provided evidence of strong interlayer interactions. To better understand the effects of interlayer interactions in $La_3Ni_2O_7$ under high pressure, we investigate a two-layer, two-orbital electron model that includes both intra- and interlayer Coulomb interaction terms within the framework of the matrix random-phase approximation. Our analysis reveals that interlayer interactions play a crucial role in determining the preferred superconducting pairing symmetry. Specifically, when interlayer interactions are included, a d_{xy}-wave pairing symmetry is favored over the $s^\pm$-wave symmetry, which was previously found to dominate in their absence. Furthermore, we find that interlayer interactions enhance interorbital pairing by incorporating contributions from all three electron pockets, which originate from both $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbital characters. This results in the emergence of nodes in the superconducting gap function - features absent in the $s^\pm$-wave state - ultimately stabilizing the d_{xy}-wave pairing symmetry.

DS 15.11 Thu 12:15 HSZ/0003

Incommensurate spin-fluctuations and competing pairing symmetries in $La_3Ni_2O_7$ — •Han-Xiang Xu[1] and Daniel Guterding[2] — [1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The discovery of superconductivity in the bilayer nickelate $La_3Ni_2O_7$ under high pressure raises key questions about the pairing symmetry and microscopic mechanism. Using a three-dimensional multi-orbital Hubbard model including all Ni 3d and O 2p states, we analyze the superconducting instability within the random phase approximation. Spin fluctuations with incommensurate wave vectors $(\pi/2, \pi/2)$ and $(7\pi/10, 7\pi/10)$ coexist and compete, leading to nearly degenerate sign-changing $s_\pm$- and $d_{x^2-y^2}$-wave pairing channels. The leading symmetry depends sensitively on pressure and the ratio of Hund's rule to Coulomb interactions. Cooperative incommensurate fluctuations stabilize a $d_{x^2-y^2}$-wave state for realistic parameters, while their competition may explain the absence of magnetic order. These findings reconcile previous contradictory results and highlight the importance of careful model construction for bilayer nickelates.

[1] H.-X. Xu and D. Guterding, arXiv:2501.05254

DS 16: Thin Film Application

Time: Thursday 9:30–12:30 Location: REC/C213

DS 16.1 Thu 9:30 REC/C213

An on-chip heating platform for localized thin-film repair, non-equilibrium microstructures, and phase control — •Nensi Toncich, Nerea Abando Beldarrain, Jacopo Simone Crippa, Henning Galinski, and Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, Switzerland

Localized on-chip heat generation and rapid thermal quenching is critical for systematic probing of phase transitions of nanofabricated systems, tailoring non-equilibrium microstructures and localized thin-film repair. Here we introduce a reactive multilayer [1] based on-chip heating platform that enables temperatures above 1000 °C, millisecond-scale heating and self-quenching rates on the order of 10^5 °C s^{-1} while preventing chemical interdiffusion. Using a diffusion-resistant, thermally conductive barrier, this platform enables three distinct, reproducible outcomes across different material systems: (i) localized melting and reflow of Au to repair electrical discontinuities, (ii) controlled microstructural evolution of Au, transforming equiaxed grains into elongated, high-aspect-ratio structures that are difficult to achieve with conventional processing, and (iii) a monoclinic-to-tetragonal phase transformation in the ZrO_2, demonstrating precise, site-specific phase engineering.

By combining ultrafast, high-temperature thermal pulses with diffusion-stable barriers, this platform offers a unique strategy for precise, on-demand modification of thin films, with broad applications in electronics, functional coatings, and nanofabrication.

[1] Toncich N. et al., J. Appl. Phys. 137(17), 2025

DS 16.2 Thu 9:45 REC/C213

Enhanced resistive switching in hybrid perovskite-MoS2 memristors — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]INN, NCSR Demokritos, 15341 Athens, Greece — [2]Physics Department, National and Kapodistrian University of Athens, Panepistimiopolis Zografos, 15784 Athens, Greece

Memristors are emerging two-terminal devices with tunable resistance states and strong potential for next-generation non-volatile memory and neuromorphic computing. Their reversible switching between high- and low-resistance states (HRS/LRS), combined with non-volatile information retention, makes them attractive for energy-efficient data storage. Metal halide perovskites have recently gained interest in thin-film memristive technologies due to their low fabrication cost, solution processability, and rich ionic dynamics, while 2D TMDs such as MoS2 provide excellent interfacial properties that modulate charge transport and defect chemistry.

We demonstrate a hybrid perovskite memristor incorporating MoS2 nanosheets, exhibiting significantly enhanced electrical performance compared to pristine devices. The MoS*-integrated device achieves endurance up to 200 switching cycles, stable retention beyond 12 000 s, and a large memory window (HRS:LRS ~100). In contrast, the pristine device shows only ~25 cycles and a window below 50. These results highlight the crucial role of TMD:perovskite interfaces in stabilizing ion-migration pathways and improving resistive-switching reliability in hybrid thin-film memristors.

DS 16.3 Thu 10:00 REC/C213

Resistive Sensor for in situ electrical monitoring during atomic layer deposition — •Lucas Rave, Colin Schormann, Stefanie Haugg, Kristian Deneke, Jun Peng, Robert Blick, and Robert Zierold — Center for Hybrid Nanostructures, University of Hamburg, Germany

Atomic layer deposition (ALD) provides exceptional coating conformality with sub-nanometer resolution, driving the new semiconductor technology node processes. Conventional in situ diagnostics, such as spectroscopic ellipsometry and quartz crystal microbalances, focus on mass and optical morphology information during deposition. However, rich electrical information remains limited. To address this, we developed an electrical in situ monitoring detector capable of resolving resistance changes for individual precursor and purge pulses. This detector contains custom-patterned titanium electrodes on Si/SiO_2 substrates, whose resistance evolution directly reflects cycle-resolved ALD surface reactions. Using this approach, we probed the deposition process for oxides, including ZnO, Al-doped ZnO (AZO), and TiO_2, capturing characteristic signatures of nucleation delays, self-limiting ligand exchange, and dopant-induced conductivity changes. Our method reveals how different precursor chemistries manifest in distinct electrical transients and provides a quantitative link between surface reaction kinetics and film evolution. The resistance-based in situ sensing offers a practical, compact, and integrable diagnostic tool for understanding and optimizing ALD processes, enabling improved control over thin-film quality in micro- and nanofabrication.

DS 16.4 Thu 10:15 REC/C213

Molecular insights into the mechanical and dynamical properties of mechanically interlocked polymer thin films — •Yang Wang[1], Andrea Giuntoli[1], and Xuzhou Yan[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, Netherlands; — [2]State Key Laboratory of Synergistic Chem-Bio Synthesis, Frontiers Science Center for Transformative Molecules, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, Shanghai 200240, P. R. China;

Mechanically interlocked networks (MINs) comprise molecular components connected by mechanical bonds, introducing topological constraints that alter deformation pathways. Coarse-grained molecular dynamics simulations are used to investigate substrate-supported and free-standing MIN thin films based on [c2]daisy chain architectures, with systematic variation of extension distance, cross-linking degree, interfacial cohesive strength, and strain rate. Strongly attractive substrates induce pronounced dynamic confinement, whereas weak adhesion leads to enhanced, free-surface-like mobility. Rings exhibit slower dynamics than axle chains, whose mobility is governed by proximity to binding sites. Pull-out and biaxial deformation simulations reveal a three-stage ring-sliding mechanism that suppresses excessive bond scission, maintains network connectivity at large strains, and delays macroscopic failure, thereby enhancing toughness and energy dissipation. These results provide molecular-level insight into MIN thin film mechanics and inform the design of adaptive, energy-dissipating polymer materials.

15 min. break

DS 16.5 Thu 10:45 REC/C213

A Pathway Towards All-Optical Light-Propagation Switching — •Jakob Lindenthal, Frithjof Pietsch, Markas Sudzius, Johannes Benduhn, and Karl Leo — TU Dresden, Institut für Angewandte Physik, Nöthnitzer Str. 61, 01187 Dresden

Dynamic switching of the light propagation is a key enabler for integrated nanophotonic circuits. Optical gratings are a widely used, versatile component for coupling light into and out of waveguides. However, their diffraction efficiency is generally set and limited well below unity by static design and process parameters such as etch depths or geometric profile quality. We experimentally demonstrate the use of a dielectric-mirror cavity for enhancing the diffraction efficiency of grating couplers beyond these intrinsic limits. Using a second counter-propagating input beam achieves near-perfect dynamic control of the coupling amplitude. The experiments are backed by analytical and numerical modeling of the cavity-enhanced diffraction efficiency and the interaction of light waves in optical-gratings multiport devices. These findings extend the concept of coherent perfect absorption (CPA) from thin absorbing layers to diffractive structures, providing an all-optical propagation switching mechanism for efficient signal input and control in compact photonic circuits and nano-optic systems.

DS 16.6 Thu 11:00 REC/C213

Investigation of Temperature-Dependent Loss Mechanisms in Tantalum and Niobium Thin-Film Coplanar-Waveguide Resonators — •Philip Schneider[1], Moritz Singer[1], Harsh Gupta[1], Benedikt Schoof[1], and Marc Tornow[1,2] — [1]TU Munich, Garching, Germany — [2]Fraunhofer EMFT, Munich, Germany

Superconducting qubits can enable scalable quantum computing. Niobium (Nb) is widely used as the base superconductor, but tantalum (Ta) can improve performance by hosting fewer two-level system (TLS) losses, especially in its native oxide. We sputter-deposited Ta and Nb thin films on silicon and studied three stacks: pure Nb, Nb with a

thin Ta cap, and Ta on a thin Nb seed layer, realizing distinct interface scenarios. The thin films were characterized by resistivity, critical temperature, RRR and X-ray diffraction. Coplanar waveguide resonators were fabricated from the $\sim$ 200 nm films to determine their internal quality factor (Q_i) in the few GHz regime. Temperature- and power-dependent measurements (100-1700 mK, -80 to -160 dBm) were fitted with a combined TLS-quasiparticle loss model to analyze loss-channels. To probe the effect of native oxide at the metal-air interfaces, the resonators were re-measured post four weeks of air exposure. In the single-photon regime at 100 mK, the average Q_i changes from 1.38×10^6 (BOE) to 1.19×10^6 (native oxide) for Nb, from 1.58×10^6 to 1.11×10^6 for Ta-capped Nb, and from 1.07×10^6 to 1.20×10^6 for Ta on an Nb seed layer. Thus, while all stacks provide Q_i in the 10^6 range, Nb-based devices degrade post oxidation, whereas the Ta dominated film remains robust and even slightly improves.

DS 16.7 Thu 11:15 REC/C213

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

Gallium phosphide (GaP) emerges as a promising material for quantum nanophotonics due to its high refractive index with low absorption in the visible, combined with a strong second-order nonlinear response and the absence of linear birefringence. Growing high-quality, single-crystalline GaP thin films on low-index substrates, however, faces challenges due to lattice and thermal mismatch, and process complexity in common epitaxial methods. Here, we demonstrate ion slicing of GaP thin films and anodic bonding onto low-index glass substrates. We fabricate GaP thin films from (100) and (110) bulk crystals with thicknesses of 760 $\pm$ 40nm. Structural and optical characterisation is used to optimise the implantation and bonding conditions with the goal of achieving high-optical quality and low absorption suitable for nanophotonic applications.

DS 16.8 Thu 11:30 REC/C213

Enhancement of photoluminescence of Er3+ ions by Mie-resonant silicon nitride metasurfaces — •Fengkai Wei[1,2], Carsten Ronning[1], Duk-Yong Choi[2], Xinru Ji[3], and Tobias Kippenberg[3] — [1]Institut für Festkörperphysik, Friedrich Schiller University Jena, Germany — [2]Research School of Physics, Australian National University, Australia — [3]Institute of Physics, Swiss Fed- eral Institute of Technology Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Mie-resonant high-index dielectric nanoparticles and metasurfaces have been suggested as a viable platform for enhancing both electric and magnetic dipole transitions of fluorescent emitters. While previous work has demonstrated the enhancement of magnetic dipolar transitions from Eu3+ ions using silicon nanocylinders, this approach was limited by silicon's strong absorption at the Eu3+ emission wavelength in visible range. Erbium features a characteristic infrared emission wavelength of 1550nm, which is widely used in telecommunication. It makes Er a good candidate of emitters in metasurface for infrared applications. This study explores the enhancement of Er3+ ions using dielectric metasurfaces composed of Mie-resonant silicon nitride metasurface. Er3+ ions were introduced into the metasurface via ion implantation. Strong room-temperature photoluminescence (PL) was only observed after annealing, which activates the ions.Maximum PL enhancement occurred at a nanocylinder radius of ˜410 nm, aligning with simulations. This study demonstrated a significant ˜40-fold PL enhancement on metasurface over a planar reference.

15 min. break

DS 16.9 Thu 12:00 REC/C213

Use of hybrid electrochromic devices for dynamic solar control in buildings — •Eleftheria Merkoulidi and George Syrrokostas — Solar Energy Laboratory, Department of Physics, University of Patras, Rion, Greece

Nowadays, the three main sectors that consume a lot of primary energy are: transport, industry, and buildings. Especially in the EU during 2023, buildings were responsible for 40% of total energy consumption, for approximately 50% of all-natural gas use, and a large portion of this energy (80%) is dedicated specifically to heating, cooling, and hot water supply for occupants. Therefore, improving the energy efficiency of buildings is critical. One effective way to improve energy efficiency is by controlling the significant energy losses (up to 60%) that occur through windows. These losses are caused by heat transfer mechanisms (conduction, convection, and radiation), as well as air leakage. A promising technological solution involves the use of adaptive chromogenic windows, such as electrochromic smart windows (ECWs). They can improve the energy efficiency of a building by modulating the sunlight and solar heat entering a building in real time, by changing their appearance (from transparent to opaque), under an applied electric field. In the present study, a way to improve their optical performance is investigated, by using a cobalt based redox electrolyte as a novel alternative to other redox couples used so far, with promising results.

DS 16.10 Thu 12:15 REC/C213

Influence of Crystal Orientation on the Oxygen Evolution Reaction in La_2NiMnO_6 Films — •Felix Tegtmeyer[1], Pia Henning[2], Shagun Thakur[2], Tobias Meyer[2], Ulrich Ross[3], Vasily Moshnyaga[4], and Jasnamol Palakkal[2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]Institute of Materials Physics, University of Göttingen, Germany — [3]4th Physical Institute, University of Göttingen, Germany — [4]1st Institute of Physics, University of Göttingen, Germany

Double perovskites such as La_2NiMnO_6 (LNMO) promise applications for catalysis in energy storage and conversion. However, investigations of the oxygen evolution reaction (OER) in LNMO remain limited to nanoparticles and powders while the effects of crystal orientation remain elusive. In this work, we study monocrystalline LNMO thin film catalysts grown by metalorganic aerosol deposition at ambient air. By controlling the facet which is in contact with the electrolyte, the influence of crystal orientation is identified. We found that the activity of LNMO films with (100) crystal orientation is enhanced by one order of magnitude compared to (111) oriented films. We attribute this to the availability of both Ni and Mn active sites for the (100) surface. Moreover, an overall enhancement of the activity is identified for higher thicknesses. In long-term chronoamperometry measurements, the LNMO film retains a high activity and excellent bulk stability while the degradation is limited to a surface-near region.

DS 17: Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)

Superconductors with record transition temperatures up to 250 K have been discovered and confirmed in hydride materials at high pressures over the last decade, enabled by major advances in both computational and experimental approaches. Density functional theory, combined with structure search algorithms and machine learning methods, enables high-throughput predictions of novel high-pressure phases. Ab initio microscopic theories, including Eliashberg theory and superconducting density functional theory, successfully predict transition temperatures of identified phases, with several predictions now confirmed experimentally. The synthesis of novel hydrides has revealed the importance of including hydrogen quantum fluctuations in theoretical predictions. Experimentally, advances in high-pressure synthesis techniques have enabled the preparation of novel hydride phases, while electrical transport measurements, tunneling spectroscopy, and magnetic studies have established a strong body of evidence for superconductivity by probing zero resistance, the superconducting gap, and magnetic response. This focus session will emphasize these breakthroughs, highlight ongoing challenges in both experiment and computation, and provide an outlook for finding high-temperature superconductors at lower and ambient pressures.

Coordinators: Philipp Gegenwart (Universität Augsburg), Matthias Vojta (TU Dresden)

Time: Thursday 15:00–18:45 Location: HSZ/0003

Topical Talk DS 17.1 Thu 15:00 HSZ/0003

Computational searches for conventional high temperature superconductivity — •Chris Pickard — University of Cambridge

First principles methods for the prediction of the structure of materials have delivered a powerful tool for generating candidate structures for comparison with experimental analytical methods. Early studies focused on the exotic properties and structures of relatively simple systems, typically the elements and binary compounds. The promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds.[1] I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, focussing on the dramatic acceleration that ephemeral data derived potentials (EDDPs) afford,[2] and their role in the uncovering of Mg_2IrH_6 as a feasible ambient pressure high temperature superconductor.[3]

[1] A.M.Shipley, M.J Hutcheon, R.J.Needs, Ch.J.Pickard, Phys. Rev. B 104, 054501 (2021)
[2] Ch.J.Pickard, Phys. Rev. B 106, 014102 (2022)
[3] K.Dolui, L.J.Conway, Ch.Heil, T.A.Strobel, R.Prasankumar, Ch.J.Pickard, Phys. Rev. Lett. 132, 166001 (2024)

Topical Talk DS 17.2 Thu 15:30 HSZ/0003

High-pressure synthesis of hydrides and their characterisation by single-crystal X-ray diffraction — •Natalia Dubrovinskaia[1] and Leonid Dubrovinsky[2] — [1]Material Physics, University of Bayreuth; Bayreuth, Germany — [2]Bayerisches Geoinstitut, University of Bayreuth, Germany

The sulfur-hydrogen, lanthanum-hydrogen, and yttrium-hydrogen systems have attracted significant interest following reports of near-ambient-temperature superconductivity in some of their high-pressure phases. Here, we present single-crystal X-ray diffraction studies of these systems, supported by density functional theory calculations, which reveal an unexpected chemical and structural diversity in S, La, and Y hydrides synthesised at 50*200 GPa. Syntheses were carried out in diamond anvil cells by laser heating S, La, LaH3, or Y together with hydrogen-rich precursors-ammonia borane or paraffin oil. The arrangements of heavy atoms in newly formed phases were determined from SCXRD data, while hydrogen contents were estimated using empirical relationships and ab initio calculations. Our study also uncovers the formation of previously unreported metal allotropes, carbides, and ternary compounds at high pressure. The complex phase diversity, variable hydrogen stoichiometries, and metallic nature of these high-pressure hydrides, as revealed by theory, highlight the challenges in identifying the superconducting phases and understanding electronic transitions in materials synthesised under extreme conditions.

Topical Talk DS 17.3 Thu 16:00 HSZ/0003

Electrical Transport Studies in bulk and thin-film hydride high-temperature superconductors — •Sven Friedemann[1], Sam Cross[1], Owen Moulding[1], Israel Osmond[1], Xiaojiao Liu[2], Annette Kleppe[2], Oliver Lord[3], and Jonathan Buhot[1] — [1]HH Wills Physics Laboratory, University of Bristol, UK — [2]Diamond Light Source Ltd., Didcot, UK — [3]School of Earth Sciences, University of Bristol, UK

Superconductivity is not restricted to low temperatures! Indeed, transition temperatures up to 260 K have been demonstrated by multiple groups in H_3S, LaH_{10}, and YH_9, at very high pressures. This is a success story of both theory and experiment. Theory has mastered accurate predictions of new superconductors and has been crucial to guide experimental efforts. Experiments have mastered many technical challenges. Together, these efforts open pathways to realise higher transition temperature at low pressures.

We present combined structural and electrical transport studies of hydride high-T_c superconductors based on our development of *in situ* synthesis, x-ray diffraction, and transport measurements in diamond-anvil pressures cells including thin-film methods for electrodes and superconducting samples. We present the characterisation of clean-limit superconductivity in H_3S and the discovery of the new superconductor La_4H_{23}. We demonstrate superconductivity in thin films of LaH_{10} with a $T_c = 250$ K consistent with bulk LaH_{10}. Our results open new avenues to study hydride high-T_c superconductors with thin-film methods.

15 min. break

Topical Talk DS 17.4 Thu 16:45 HSZ/0003

Near room-temperature conventional superconductivity in hydrogen-rich compounds at high pressures: Experimental evidences — •Vasily Minkov — Max Planck Institute for Chemistry, Mainz, Germany

The pioneering discovery of superconductivity in hydrogen sulfide (H3S) with a record Tc of 203 K at 150 GPa by M. Eremets et al. had a profound impact on the field. It validated the concept of high-Tc conventional superconductivity in hydrides and triggered an intense wave of research. Subsequent studies revealed that other hydrides - such as LaH10 and YH9 - exhibit Tc values approaching 250 K, bringing the field closer than ever to room-temperature superconductivity. Despite the experimental challenges associated with micrometer-sized samples confined in diamond anvil cells, superconductivity in these compounds has been demonstrated using multiple independent techniques. Electrical four-probe measurements provide clear resistive transitions, while recent advances in high-pressure magnetometry enable direct detection of magnetic field screening and flux expulsion. We have further developed a method to probe trapped magnetic flux in hydrides at high pressure. The distinct behavior of trapped flux generated under ZFC and FC conditions provides strong evidence for superconductivity. Furthermore, the recent adaptation of electron tunneling spectroscopy to extreme pressures offers microscopic insight into the pairing mechanism and enables direct characterization of the superconducting gap structure in the high-temperature hydride superconductors.

Topical Talk DS 17.5 Thu 17:15 HSZ/0003

Predictive T_c Calculations in Hydride Superconductors — •Christoph Heil — Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

The discovery of high-T_c superconductivity in compressed hydrides has sparked a surge of theoretical predictions, yet reported critical temperatures for identical structures can differ by tens of Kelvin or more. These discrepancies reflect differences in how lattice dynamics, electronic structure, and Coulomb repulsion are treated. In this talk, we will present first-principles workflows designed to make Tc calculations both more transparent and more predictive.

We combine anharmonic lattice dynamics with full-bandwidth isotropic and anisotropic Migdal-Eliashberg calculations (IsoME and EPW) that retain the full electronic density of states, and we incorporate Coulomb repulsion via screened interactions obtained from first principles rather than an empirical μ^*. This framework allows us to systematically compare different approximation levels and to quantify how each approximation affects T_c.

Using case studies from high-pressure hydrides, we will demonstrate when simplified treatments remain adequate and when anharmonic effects, full-bandwidth electrons, and first-principle determination of Coulomb screening become essential for quantitative accuracy. I will provide practical guidelines for reliable, reproducible T_c predictions and discuss how rigorous superconductivity calculations complement crystal-structure prediction efforts in the search for new superconductors.

DS 17.6 Thu 17:45 HSZ/0003

^{1}H-NMR investigations of bulk superconductivity in superhydrides using Lenz lenses — •F. Bärtl[1,2], D. Zhou[3], T. Helm[1], S. Luther[1], H. Kühne[1], J. Wosnitza[1,2], and D. Semenok[3] — [1]HLD-EMFL, HZDR, Dresden — [2]IFMP, TUD, Dresden — [3]HPSTAR, Beijing

The discovery of near-room-temperature superconductivity at ultrahigh pressures in superhydrides has kindled intensive research activities in the past years. However, the need to use diamond-anvil cells (DACs) for the synthesis and study of such superconductors limits the number of available experimental techniques. Nuclear magnetic resonance (NMR) spectroscopy is a key technique to study the bulk properties of superconducting materials, but it usually requires sample masses of several milligrams. Here, we present our ^{1}H NMR measurements of several superhydride preparations, using Lenz lenses, which act as magnetic-flux transformers in the NMR experiment and enable the investigation of samples with masses in the microgram range in the sample chamber of DACs. We observe several features that evidence the bulk nature of the superconducting transition in the superhydrides, the most prominent being the suppression of the ^{1}H nuclear spin-lattice relaxation rate $1/T_1T \propto D(E_\mathrm{F})^2$. Furthermore, we report on the systematic occurrence of a rate enhancement in the regime of the superconducting transition, which is reminiscent of a Hebel-Slichter-like peak.

DS 17.7 Thu 18:00 HSZ/0003

Above-room-temperature superconductivity in substituted LaH_x superhydride — •Stanley Tozer and Audrey Grockowiak — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, 01069 Dresden, Germany

We have synthesized a higher order La-based superhydride with initial superconducting transition temperature of 294 K that, when heated, morphed into a higher order system with a T_c ^{onset} of 556 K and a transition width of approximately 120 K [1]. The x-ray and the electrical transport data support one another with regard to the pressure measured, and the inhomogeneous nature of the synthesis that resulted in a substituted higher order La-based superhydride in close proximity to FIBed electrodes with a broad multi-phase, irreversible transition and non-zero background resistance below T_c. The electric leads embedded in our 'crucible' probe a pathway through this inhomogeneous growth, a very small portion of which is the superconductor of interest. We have used informed growth to reproduce the initial result in a range of pressures lower than allowed for the binary LaH_{10}. A multi-probe approach is being implemented to address growth-to-growth variations and follow the transformation of the initial 294 K superconductor. This will provide an understanding of this new class of superconductor that begs the question as to the upper limit of superconductivity in the superhydrides and whether BCS theory can describe them.

[1] A.D. Grockowiak et al., Electronic Materials 2, (2022)
[2] doi.org10.3389/femat.2022.837651

DS 17.8 Thu 18:15 HSZ/0003

Search for Room-temperature Superconductivity in the La-Sc-H System — •Dmitrii V. Semenok[1], Ivan A. Troyan[2], Di Zhou[1], and Viktor V. Struzhkin[1,3] — [1]Center for High Pressure Science & Technology Advanced Research, Bldg. 8E, 10 Xibeiwang East Rd, Beijing, 100193, China — [2]private — [3]Center for High Pressure Science & Technology Advanced Research, 1690 Cailun Rd, Bldg 6, Shanghai 201203, China

One of the highlights of 2025 in the field of hydride superconductivity was the announcement of the experimental discovery of room-temperature superconductivity in the fully ordered ternary polyhydride P6/mmm-$LaSc_2H_{24}$ at around 260 GPa [1]. We performed a DFT analysis of intermetallic compound formation in the La-Sc system with a view to modifying the synthetic procedure, and calculated parameters of the superconducting state of the isostructural P6/mmm-La_3H_{24} and P6/mmm-Sc_3H_{24} at 300 GPa. Attempts to experimentally reproduce the synthesis of $LaSc_2H_{24}$ from the $LaSc_2$ alloy (with a careful selection of the homogeneity region of this alloy's composition) at 264-280 GPa have not yet resulted in the detection of any traces of superconductivity between 255 K and 295 K in the corresponding hydride. In my report, I will show the results of additional experimental attempts to reproduce [1], planned for January-February 2026.

[1] Y. Song et al., arXiv: 2510.01273 (2025).

DS 17.9 Thu 18:30 HSZ/0003

Computational modeling of disordered hydride superconductors — •Pedro Nunes Ferreira[1], Luiz Tadeu Fernandes Eleno[2], and Christoph Heil[1] — [1]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010, Graz, Austria — [2]Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena, Brazil

Designing and optimizing novel hydride superconductors requires methods that accurately treat realistic chemical disorder. In this talk, I will present an ab initio thermodynamic framework, the extended generalized quasichemical approximation (EGQCA), tailored to the modeling of superconducting alloys, especially high-T_c superhydrides. EGQCA enables the prediction of any computationally accessible property, such as T_c and electron-phonon coupling, as a function of composition using only a small set of supercell calculations, making it particularly well suited for complex hydrogen-rich materials. I will illustrate its capabilities with applications to high-T_c superhydrides at high pressure, as well as defective hydrides stabilized at ambient pressure. Finally, I will discuss how EGQCA opens the door to high-throughput design and screening of disordered superconductors, with the potential to significantly advance hydride superconductivity research.

DS 18: Spins in Molecular Systems

Time: Thursday 15:00–17:30 Location: REC/C213

DS 18.1 Thu 15:00 REC/C213

The forgotten sister of the CISS effect: spin polarization induced via proximity of adsorbed chiral molecules — •Franziska Schölzel[1], Aybüke Gülkaya[2], Dominik Hornig[1], Rico Ehrler[1], Lokesh Rasabathina[1], Aleksandr Kazimir[3], Christina Lamers[3], Olav Hellwig[1], Michael Mehring[1], Shuxia Tao[2], and Georgeta Salvan[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Eindhoven University of Technology, Eindhoven, the Netherlands — [3]Leipzig University, Leipzig, Germany

Within the past years a new research field around chirality induced spin selectivity (CISS) has emerged and gains increasing attention. The central part is often played by complex chiral or helical molecules; ferromagnetic, gold capped, sometimes structured substrates and electrical transport measurements [1]. An aspect most often forgotten within this framework is the effects static equivalent [2]. We observed the Spin Polarization Induced via the Proximity of Adsorbed Chiral Molecules (SPIPAC) effect in nickel thin films for various chiral molecules. This study probes the resulting magneto-optical signal of the Ni substrate using Circular Dichroism spectroscopy. Furthermore, the impact of film thickness of the substrate, molecule density on the surface and the chirality of the molecules is explored. [1] B. Bloom et al., Chem. Rev. 124, 4, 1950-1991 (2024) [2] O. Ben Dor et al., Nat Commun 8, 14567 (2017)

DS 18.2 Thu 15:15 REC/C213

Understanding interface-controlled CISS-MR (magnetoresistance) via electric dipole inversion using ambient STM — •T. N. Ha Nguyen[1], Lech Tomasz Baczewski[2], Aleksandr Kazimir[3], Christina Lamers[3], and Christoph Tegenkamp[1] — [1]Analysis of Solid Surfaces, Nanostructures and Quantum Materials, Technische Universität Chemnitz, Germany — [2]Reichenhainerstr., 70 — [3]Institute for Drug Discovery, Medical Faculty University of Leipzig, Leipzig, Germany

Recent studies have highlighted the significant influence of electric dipole moment orientation in chiral molecules on spin polarization. When chiral molecules with strong dipole moments adsorb onto a surface, their orientation breaks the interfacial symmetry, leading to enhanced spin-polarized currents. Using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we measured spin-polarized electron transport through polyalanine molecules, which possess substantial dipole moments. Notably, inverting the dipole moment while maintaining the molecule*s chirality results in a reversal of the chiral-induced spin selectivity magnetoresistance (CISS-MR). Our findings not only highlight the crucial role of electric dipole moments in chiral molecules but also provide insights into the CISS mechanism, particularly regarding the interface effect.

DS 18.3 Thu 15:30 REC/C213

Effect of adsorbed chiral molecules on the magnetic properties of skyrmion-hosting multilayers — •Mariam Hassan[1,2], Ivan Saldatov[3], Lokesh Rasabathina[4], Franziska Schölzel[1,2], D.R.T Zahn[1,2], Olav Hallwig[1,4], and Georgeta Salvan[1,2] — [1]Research Center for Materials, MAIN, Chemnitz University of Technology, Germany — [2]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Germany — [3]Institute for Metallic Materials, IFW, Dresden — [4]Functional Magnetic Materials, Institute of Physics, Chemnitz University of Technology, Germany

Chirality-induced spin selectivity (CISS) and Magnetism Induced by Proximity of Adsorbed Chiral molecules (MIPAC) effects are phenomena that caught significant interests over the last few decades because of the large spin polarizations generated by organic molecules and the alteration of the surface's magnetism upon the adsorption of chiral molecules respectively [1,2]. On the other hand, magnetic skyrmions have emerged as a promising path for next-generation information storage and processing technologies. Thus, tuning skyrmion properties is of increasing interest for application in future spintronic devices. In light of the CISS and MIPAC effects, the use of chiral molecules might represent an attractive approach to address the challenge of tuning skyrmion properties [3]. In this work, we aim to investigate how adsorbed chiral molecules interact with magnetic skyrmions that are stabilized in [Co/Ni]N ferromagnetic multilayers with PMA. We observe that the adsorbed chiral molecules locally change the magnetic properties of the film, affecting the density of skyrmion nucleation sites.

DS 18.4 Thu 15:45 REC/C213

Self-Assembly of Helical Molecular Monolayers Using a Coarse-Grained Chiral Patchy Model — •Hadis Ghodrati Saeini[1], Faezeh Shabani[1], Sibylle Gemming[1], Christoph Tegenkamp[1], Florian Günther[2], and Jeffrey Kelling[1,3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]São Paulo State University, Rio Claro, Brazil — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The Chiral-Induced Spin Selectivity (CISS) effect makes helical molecules promising for spintronic applications, yet their surface self-assembly remains poorly understood due to experimental and computational constraints. Although Density-Functional Tight-Binding (DFTB) potentials accurately describe polyalanine (PA) α-helix SAMs, their high computational cost limits large-scale and kinetic investigations.

We introduce a coarse-grained chiral patchy model parameterized to fit the PA-specific DFTB potential, capturing its essential chiral symmetry and interaction features while remaining computationally efficient. Validation is achieved by comparing low-energy configurations obtained from annealing Monte Carlo simulations using the DFTB-based potential with dynamic pathways from coarse-grained molecular dynamics. Dynamic simulations made feasible by this model successfully reproduce the final assembled morphologies and allow explorations of potential metastable states, demonstrating its reliability and versatility for studying the kinetics of helical molecular self-assembly.

DS 18.5 Thu 16:00 REC/C213

Exploring the Origins of Helical Bundle Stability and Their Role in the CISS Effect — •Faezeh Shabani[1], Sibylle Gemming[1], Georg Kuenze[2], Paul Kluge[2], and Florian Guenther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Universität Leipzig, Leipzig, Germany — [3]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Helical bundles provide a highly regular and tunable chiral environment, making them ideal model systems for investigating the principles of the CISS effect and exploring possibilities for generating electronic hyperpolarization through (super)helical geometries. Beyond their relevance to chiral-induced spin selectivity, helix bundles also play important roles in nature: they consist of two or more α-helices supercoiled around a central axis and function as essential structural motifs in many biological systems. In this talk, we explore these characteristics using DFTB+ calculations. This computational approach allows us to analyze the energetic origins of specific bundling motifs, assess the role of dispersion interactions, and ultimately understand why certain helix bundle architectures are favored in nature.

15 min. break

DS 18.6 Thu 16:30 REC/C213

Unwinding the Helicity-Driven Electronic Properties in Polyproline I and II Chains — •Saba Arshad, Faezeh Shabani, and Sibylle Gemming — TU Chemnitz, Chemnitz, Germany

Polyproline is a polypeptide that adopts two distinct helical conformations, polyproline I (PPI) and polyproline II (PPII), with identical primary sequence but markedly different helicities and structural behavior, providing a valuable platform for examining electronic properties and their potential impact on CISS (Chirality-Induced Spin Selectivity) effects. Here, we employed density-functional approaches for chains with different numbers of monomers to investigate how helical geometry influences the electronic properties of both conformers. Our results reveal significant differences in the HOMO-LUMO gap and density of states between PPI and PPII, with the gap consistently narrowing as additional monomers are incorporated. Dipole moments calculated for chains of increasing length display distinct scaling trends for PPI and PPII helices, highlighting how both chain length and topology govern emerging molecular electronic applications.

DS 18.7 Thu 16:45 REC/C213

Modelling spin particles in an infinite helical box —

Alex Mureşan[1,2], Fabian Prasse[1], and •Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Calculating the electronic states of a quantum mechanical particle in a potential well with infinitely high walls is probably the most readily accessible, still analytically solvable textbook example of quantisation via spatial confinement. As such, it is an ideal starting point for including additional terms to the Hamiltonian in order to adapt the model to a specific experimental setting, e.g. by introducing multiple particles or external fields. Here we present an extension that assumes an externally given spatial modulation of the potential well with helical characteristics as boundary condition. We derive analytical solutions for the motion of classical, Newtonian particles on a helical path, for charged Schrödinger-type quantum particles in a one-dimensional helical confinement, and quantum-mechanical spin 1/2-particles in a helical spin-orbit-split environment, which is encountered in investigations of the chirality-induced spin selectivity effect. We show that the model extension steps successively refine the eigenspectra of the simplest case, and that the spin-orbit interaction term leads to an extra splitting within the helical confinement.

Invited Talk DS 18.8 Thu 17:00 REC/C213

Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces — •Frank Ortmann — Technical University of Munich, Munich, Germany

Understanding charge, exciton and spin dynamics in molecular systems is critical for advancing organic semiconductor-based technologies. We present insights from our work addressing distinct yet complementary aspects of these phenomena for organic-electronics materials. First, we explore charge-transfer dynamics in electron-phonon coupled model systems, identifying regimes such as polaron transport and transient localization, emphasizing their seamless transitions across vibrational modes and temperatures. Second, a comparative analysis of the Matrix Product State (MPS) and Multilayer Multiconfiguration Time-Dependent Hartree (MCTDH) methods demonstrates their efficacy in modeling non-adiabatic exciton dissociation, revealing specific sensitivities to electronic-vibrational entanglement in complex systems. Lastly, we introduce current work toward a general quantum mechanical treatment of spin transport in donor-acceptor systems. These works underline the theoretical advances in capturing the interplay of various degrees of freedom in molecular optoelectronics and spintronics.

DS 19: Members' Assembly

Time: Thursday 17:45–18:30 Location: REC/C213

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

DS 20: Poster

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

DS 20.1 Thu 18:30 P2

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

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

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

DS 20.2 Thu 18:30 P2

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

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

DS 20.3 Thu 18:30 P2

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

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

DS 20.4 Thu 18:30 P2

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

Architectural glass facades worldwide typically utilize solar-control coatings deposited in inline magnetron sputter coaters to prevent buildings from excess solar heating. To use the electricity-generating potential of these facades, we aim to enable the glass industry to integrate photovoltaic functionality into their glazing using existing production lines. This requires a semi-transparent, fully sputtered thin-

film solar cell. As a first step, here we demonstrate sputtered ultra-thin germanium absorber layers for semi-transparent solar cells. We compare their optoelectronic properties and their microstructure with established reference layers deposited by plasma-enhanced chemical vapor deposition (PECVD) and identify sputter-process conditions that yield germanium absorbers with PECVD-comparable properties suitable for device integration. We present a sputtered germanium layer built into a solar cell, which delivers a power conversion efficiency of 2.8%. These results demonstrate that sputtered germanium is a viable absorber for thin-film photovoltaics and represent an important step towards an industrially sputtered semi-transparent solar cell for window applications.

DS 20.5 Thu 18:30 P2

Enhanced Ferroelectric Behavior in NH4Cl-Doped SnO2/Perovskite Multilayer Memristors — •Katerina Maskanaki[1], Evangelos Evangelou[1], and Anastasia Soultati[2,3] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Institute of Nanoscience and Nanotechnology (INN), National Center for Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece — [3]Department of Electrical & Computer Engineering, Hellenic Mediterranean University (HMU), Heraklion 71410, Crete, Greece

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

DS 20.6 Thu 18:30 P2

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

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

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

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

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

DS 20.7 Thu 18:30 P2

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

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

DS 20.8 Thu 18:30 P2

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

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

DS 20.9 Thu 18:30 P2

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

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

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

This work presents the current progress in the development of such a sensor. Barium Titanate (BaTiO3) was selected as the piezoelectric material due to its high piezoelectric coefficient and more environmentally friendly profile compared to PZT. The coating was successfully applied using two different methods: sol-gel dip coating and pulsed laser deposition. Potential application areas and opportunities for further design optimization are also discussed.

DS 20.10 Thu 18:30 P2

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

Precise positioning is a never-ending goal in both fundamental science and technology. Conventional position-sensitive detectors (PSDs), which rely on lateral photoelectric effects in semiconductor junctions, are inherently restricted in operating temperature and are often unsuitable for detection beyond the optical regime. Here, we present a new detector architecture, the thermoelectric-based position-sensitive detector (T-PSD), that extracts spatial information solely from heat con-

duction and thermoelectric conversion. Specifically, the device incorporates an ALD-deposited Al-doped ZnO (AZO) thermoelectric thin film on an isotropic substrate, where Seebeck voltages measured across multiple electrodes encode the position of an incident heat spot. It can detect single heat spots arising from various energy sources, including electromagnetic radiation, electrons, and macroscopic mechanical heat. The thin-film design enables sub-micrometer spatial resolution in 1D configurations, while a two-ratio voltage decoding scheme provides robust and intensity-independent localization in 2D devices. Furthermore, the T-PSD exhibits broad temperature compatibility and is particularly well suited for high-energy beams, which remain challenging to localize with existing PSD technologies.

DS 20.11 Thu 18:30 P2

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

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

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

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

DS 20.12 Thu 18:30 P2

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

In recent years, energetic heavy ions have been used to modify the physical properties of various materials [1]. In this study, we investigate the influence of irradiation of molybdenum trioxide (MoO3) thin films with MeV ions of various parameters [2]. The films were deposited on fused silica using thermal evaporation technique. After irradiation, the films were characterized using optical spectroscopy and XRD techniques, showing the effectiveness of ion-irradiation in tuning the films optical and structural properties by varying ion beam parameters. This is highly important for the design of advanced metal oxide materials for sensing, switching, and energy applications.

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

DS 20.13 Thu 18:30 P2

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

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

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

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

DS 20.14 Thu 18:30 P2

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

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

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

DS 20.15 Thu 18:30 P2

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

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

DS 20.16 Thu 18:30 P2

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

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

DS 20.17 Thu 18:30 P2

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

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

DS 20.18 Thu 18:30 P2

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

Hexagonal boron nitride (h-BN) offers multiple interesting applications as a component in heterostructures with other 2D materials, for example as a passivation layer or a tunnel barrier in electronics. However, the synthesis of large-scale high quality h-BN required for such applications remains challenging, and the vast majority of the van der Waals heterostructures having h-BN as a building block are still prepared using mechanically exfoliated h-BN flakes.
To serve as a substrate for large-scale h-BN grown by molecular beam epitaxy (MBE), in this work, we investigate the synthesis of Ni films on Al_2O_3(0001) and MgO(111) using magnetron sputtering. The structure and morphology of the Ni films is characterized using X-ray diffraction (XRD), atomic force microscopy (AFM) and electron backscatter diffraction (EBSD). The structural quality of the Ni films is improved by systematically varying experimental parameters such as substrate temperature, sputtering power, film thickness and the post-growth annealing temperature, finally resulting in single crystalline Ni films with (111) orientation only.

DS 20.19 Thu 18:30 P2

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

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

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

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

DS 20.20 Thu 18:30 P2

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

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

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

DS 20.21 Thu 18:30 P2

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

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

DS 20.22 Thu 18:30 P2

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

Bulk Niobium cavities are the state-of-the-art option to realizes high-performing linear particle accelerators. To achieve even better performance and lowering operational costs, a thin film approach with different superconducting materials is necessary. Nb3Sn coatings are

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

DS 20.23 Thu 18:30 P2

Surface Investigations of Ga-polar wz-GaN Grown by Plasma Assisted MBE — •Abdul Qadir Shabaz[1,2], Anees Ul Hassan[1,2], Fabian Ullmann[1,2], and Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

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

DS 20.24 Thu 18:30 P2

Bonding and properties in NiTe-$NiTe_2$: Transition from normal metal to Dirac semimetal — •Christian Stenz[1], Kethusan Karunanathan[1], Paul Zhuromskyy[1], Kijoon Cheong[1], Tim Bartsch[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

We investigate the evolution of bonding and electronic properties across the NiTe-$NiTe_2$ system, focusing on the transition from conventional metallic behavior in NiTe to topological Dirac semimetallicity in $NiTe_2$. NiTe exhibits isotropic bonding between Ni d- and Te p-electrons, characteristic of a normal metal. In contrast, $NiTe_2$ forms a layered structure with a pseudo van-der-Waals gap and weak Te p-p interactions, hosting Dirac nodes near the Fermi level that give rise to non-trivial topological surface states and linear magnetoresistance. By tuning the Ni content in sputtered thin films, we control the interlayer coupling mediated by Ni d-electrons, enabling systematic exploration of the transition between these bonding regimes. Using density functional theory and tight-binding calculations, we analyze how additional d-electrons influence the band structure, Berry curvature, and Dirac cone formation in $NiTe_2$. Correlations between these electronic changes and material properties - such as optical and electrical conductivity, linear positive magnetoresistance, emergence of soft anharmonic bonds and bond rupture behavior - are examined.

DS 20.25 Thu 18:30 P2

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

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

DS 20.26 Thu 18:30 P2

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

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

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

References: [1] L. M. Vicente-Arche et al., Phys. Rev. Mater. 5, 064005 (2021).

DS 20.27 Thu 18:30 P2

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

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

DS 20.28 Thu 18:30 P2

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

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

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

DS 20.29 Thu 18:30 P2

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

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

DS 20.30 Thu 18:30 P2

From Localised to Delocalised Charge Carriers: An Optical Investigation on Metal-Insulator Transitions — •Thomas Schmidt[1], Navjot Bamrah[2], Liron B. Michael[2], Ricardo P. M. S. Lobo[3], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany — [3]LPEM, ESPCI Paris, CNRS, PSL University, 75231 Paris, France

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

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

DS 20.31 Thu 18:30 P2

Investigating the Anisotropy of Optical Phonons in Ultrafast Optical Pump-Probe Experiments — •Felix Nöhl[1], Felix Hoff[1], Jonathan Frank[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

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

DS 20.32 Thu 18:30 P2

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

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

DS 20.33 Thu 18:30 P2

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

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

DS 20.34 Thu 18:30 P2

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

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

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

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

DS 20.35 Thu 18:30 P2

A Kramers-Kronig Consistent, Parameter Free, Probabilistic Dielectric Function Model — •Noah Stiehm[1,2], Stefan Krischok[1], Rüdiger Schmidt-Grund[1], and Jana de Wiljes[2] —

[1]Technische Physik I, TU Ilmenau, Germany — [2]Mathematics of Data Science, TU Ilmenau, Germany

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

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

DS 20.36 Thu 18:30 P2

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

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

DS 20.37 Thu 18:30 P2

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

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

DS 20.38 Thu 18:30 P2

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

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

DS 20.39 Thu 18:30 P2

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

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

DS 20.40 Thu 18:30 P2

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

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

DS 20.41 Thu 18:30 P2

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

Emerging memory devices are a possibility to reduce electricity expenditure in the future compared to established complementary metal-

oxide-semiconductors CMOS. For instance the Mottronic is based on a topotactic phase transition TPT associated with a metal-insulator transition MIT, instead of a manipulation of charges like in semiconductors. This might allow a further miniaturization of devices.

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

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

DS 20.42 Thu 18:30 P2

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

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

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

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

[1] A. A. Rybkina et al., Phys. Rev. B 104 (2021) 155423.
[2] N. Briggs et al., Nanoscale 11 (2019) 15440. 4.
[3] M. Kruskopf et al., 2D Mater. 3 (2016) 041002.

DS 20.43 Thu 18:30 P2

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

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

DS 20.44 Thu 18:30 P2

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

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

DS 20.45 Thu 18:30 P2

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

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

DS 20.46 Thu 18:30 P2

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

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

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

DS 20.47 Thu 18:30 P2

Modeling intermolecular interactions and ordered packing in self-assembled monolayers of polyalanine α-helices — Hadis Ghodrati Saeini[1], Thi Ngoc Ha Nguyen[1], Christoph Tegenkamp[1], Sibylle Gemming[1], Jeffrey Kelling[2], and •Florian Günther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]São Paulo State University, Rio Claro, Brazil

Polypeptide molecules are attracting attention as promising candidates for electronic spin-filters due to the phenomenon of chiral-induced spin selectivity (CISS). This motivates substantial research to characterize the structural and electrical properties of self-assembled monolayers

(SAMs) of peptide helices, for example, polyalanine (PA) α-helices. In this work, we aim to characterize the intermolecular interactions governing PA-SAM film formation. We developed an empirical potential that models the interaction between two isolated helices, derived using the density functional-based tight-binding (DFTB) method. This potential allowed us to simulate the most energetically favorable arrangements in SAM films via a Monte Carlo approach employing simulated annealing and the Metropolis algorithm. Statistical analysis of the relative positioning of adjacent molecules enabled us to classify the degree of frustration in the films. For enantiopure systems, a frustration-free arrangement was found, yielding a perfect hexagonal lattice. For mixtures of chiralities, the results showed parallel-aligned domains of differently handed helices. Both findings are in excellent agreement with experimental works.

DS 20.48 Thu 18:30 P2

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

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

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

DS 20.49 Thu 18:30 P2

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

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

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

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

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

DS 20.50 Thu 18:30 P2

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

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

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

DS 20.51 Thu 18:30 P2

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

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

DS 20.52 Thu 18:30 P2

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

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

DS 21: Optical Analysis of Thin Films

Time: Friday 9:30–12:30 Location: REC/C213

DS 21.1 Fri 9:30 REC/C213

From Semiconductors to Quantum Materials: Ultrafast Optical Signatures Across Chalcogenide Classes — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Optical pump probe spectroscopy provides a powerful means to investigate and compare ultrafast dynamics in diverse material classes, ranging from covalently bonded semiconductors to quantum materials. In this study, we contrast the optical and structural responses of sesquichalcogenides like In2Te3 films with those of quantum materials such as Bi2Te3 or Sb2Te3. Femtosecond pump probe and complementary spectroscopic analyses reveal that In2Te3 exhibits remarkably stable optical and vibrational properties across a wide thickness range, attributed to its predominantly covalent bonding network. In contrast, quantum materials based on Bi or Sb display pronounced thickness-dependent responses and strong coupling between coherent phonons and electronic states. These materials demonstrate tunable coherent lattice motions through variations in pump fluence, polarization, and pulse sequencing, offering routes for ultrafast manipulation of quantum states. The comparison highlights a clear distinction between structurally robust semiconducting chalcogenides and highly responsive quantum materials. Together, these findings delineate how bonding character and electronic topology govern ultrafast optical behavior.

DS 21.2 Fri 9:45 REC/C213

Orientation-Dependent Near-Field Infrared Properties of a Chiral SURMOF — •Nadine von Coelln[1], Ana C. Fingolo[2], Benedikt Zerulla[3], Marjan Krstić[4], Christian Huck[1], Carsten Rockstuhl[3,4], Christof Wöll[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Functional Interfaces — [3]Institute of Nanotechnology — [4]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany

Chiral surface-anchored metal organic frameworks (SURMOFs) are promising candidates for enantioselective separation, molecular sensing and optoelectronic applications with circularly polarized light. Given the large possible design space, it is highly important to understand their spectral response and to be able to predictively model SURMOF structures to determine interesting candidates for experimental screening. In this work, we employ infrared scanning near-field optical microscopy (IR-SNOM) to probe anisotropic infrared properties. Crystallites with two distinct molecular orientations exhibited pronounced differences in their near-field infrared spectra. A controlled manipulation of crystal orientation confirmed that molecular orientation is the origin of these spectral differences. A multi-scale modeling approach, spanning single MOF unit cell simulations to thin-film Maxwell scattering calculations, was validated as it reproduced the spectral signatures and strong orientation sensitivity of the material [1].

[1] A. Fingolo, N. von Coelln et al., *Adv. Funct. Mater.* e24088 (2025).

DS 21.3 Fri 10:00 REC/C213

Pressure-dependent photoluminescence and Raman spectra of GeSn alloys — •Stefan Zollner[1], Sonam Yadav[1], Meghan A. Worrell[1], Preston T. Webster[2], Rigo A. Carrasco[2], and Perry C. Grant[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]AFRL Space Vehicles Directorate, Albuquerque, NM, USA — [3]Arktonics LLC, Fayetteville, AR, USA

Optical spectra of $Ge_{1-x}Sn_x$ alloys (x<10%) grown on Si by chemical vapor deposition were acquired in a gas-membrane diamond anvil cell at pressures up to 10 GPa. The Si substrate contracts hydrostatically under pressure and imposes a biaxial stress on the thin epitaxial layer. The tetragonal distortion of the layer can be calculated from the bulk modulus of the substrate and the elastic constants of the layer. Room temperature Raman spectra of bulk Ge with 532 nm excitation show a parabolic blueshift from 300 cm^{-1} at atmospheric pressure to 335 cm^{-1} at 10 GPa. The blueshift due to pressure is linear and slightly larger for Ge on Si. We also acquired photoluminescence spectra of $Ge_{1-x}Sn_x$ alloys as a function of temperature and pressure. We observe a blueshift of the infrared $Ge_{1-x}Sn_x$ emission at 10 K of 46 meV/GPa which quenches at 0.6 GPa. For MWIR III/V multiple quantum wells, the blueshift is larger at 77 meV/GPa and the emission quenches at 1.3 GPa.

15 min. break

DS 21.4 Fri 10:30 REC/C213

VIPR: A Modular Machine Learning Framework for Inverse Problems with Application to Reflectometry — •Sascha Creutzburg[1,6], Jeyhun Rustamov[2], Alexandros Koutsioumpas[4], Jens Bornschein[1,6], Marina Ganeva[4], Stefan Häusler[4], Bernd Helm[1,6], Alexander Hinderhofer[5], Mykhailo Levytskyi[4], Valentin Munteanu[5], Robert Juzak[1,6], Vedhas Pandit[2], Frank Schreiber[5], Jeffrey Kelling[2,3], and Nico Mothes[1,6] — [1]Helm & Walter IT-Solutions GmbH, Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Chemnitz University of Technology — [4]Jülich Centre for Neutron Science, Heinz Maier-Leibnitz Zentrum — [5]University of Tübingen — [6]Saxony.AI

Ambiguous inverse problems are ubiquitous in experimental physics, where multiple parameter configurations can reproduce the same measurement and classical iterative approaches are often too slow for online analysis. We present the VIPR framework, a modular machine-learning approach for such problems in thin-film reflectometry. Its reflectometry plugin for X-ray and neutron reflectometry combines three approaches: (i) Reflectorch for fast parameter estimation, (ii) prior-amortized neural posterior estimation, and (iii) neural spline flows to capture multimodal posteriors and reveal alternative plausible structures. VIPR features streaming mode for near-real-time beamline feedback and is deployed at Heinz Maier-Leibnitz Zentrum for routine analysis. The framework integrates seamlessly into existing workflows and can be extended to other inverse problems via its plugin architecture. Code: https://codebase.helmholtz.cloud/vipr/vipr-framework

DS 21.5 Fri 10:45 REC/C213

Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures: Uncovering a Structural Phase Change in 2D Polar Ga — •Jakob Henz[1], Arpit Jain[2], Joshua A. Robinson[2], Su Y. Quek[3], and Ursula Wurstbauer[3] — [1]University of Münster — [2]Center for 2DLM, PennState University — [3]Centre for Advanced 2D Materials, National University of Singapore

2D polar metals are a class of atomically thin 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms are intercalated between a graphene and 6H-SiC interface[1]. This results in a large area, stable 2D metal film with a bonding gradient ranging from covalent over metallic to a vdW-interaction within only two to three atomic layers[2].

Here, we use cryogenic spectroscopic imaging ellipsometry to investigate the temperature dependent light-matter interaction in bilayer 2D polar gallium down to 1 K.

Contrary to theoretical expectations[1], we find a change in the local dielectric response of the material from a homogenous behavior at room temperature to a heterogenous regime at low temperatures, characterized by two absorption peaks localized to distinct surface areas on the sample[3]. This change is interpreted to indicate a structural phase transition in the material.

1 N. Briggs et al., Nat. Mater. **19**.6, 637-643 (2020).
2 M. A. Steves et al., Nano Letters **20**.11, 8312-8318 (2020).
3 J. Henz et al., in preparation (2025).

DS 21.6 Fri 11:00 REC/C213

Adsorption-Driven Vibrational and Electronic Changes on Cu(110) — •Sarang Bhasme, Mariella Denk, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

Surface resonant Raman spectroscopy (SRRS) provides a sensitive approach for probing phonons and electron-phonon interactions on metal surfaces through resonant coupling to the surface electronic states.[1] In this work, SRRS combined with reflectance difference spectroscopy is employed to investigate adsorption induced modifications of the vibrational response of Cu(110) under ultra-high-vacuum conditions. Time-resolved SRRS measurements during controlled CO and Oxygen

exposure reveal systematic evolution in phonon-related features, indicating changes in surface electronic structures and scattering pathways as adsorption progresses. These data enable comparative assessment of molecule-specific interactions and adsorption dynamics on the same surface.

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

15 min. break

DS 21.7 Fri 11:30 REC/C213

Refining the Tanguy dispersion model for strong direct interband interactions — •Beáta Hroncová and Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

In semiconductors, absorption near the band gap energy is dominated by electron valence-to-conduction band transitions. Exciton formation effectively reduces the band gap and enhances the absorption coefficient. A sharp excitonic peak corresponding to this bound state is observed in the spectral function, especially at low temperatures and low carrier concentrations [1]. At higher temperatures, the bound state is broadened and the peak disappears, but the Sommerfeld enhancement of the absorption persists.

A dispersion model of Wannier–Mott excitons with a screened Coulomb potential was derived by Tanguy [2]. However, if the band gap is small, the interactions between the conduction and valence bands are more prominent. This leads to deviations from the parabolic band curvature, and the effective mass approximation used for the calculation of the excitonic spectra is no longer accurate.

We study the dielectric response of InAs and InSb near the band edge measured by spectroscopic ellipsometry in a wide range of temperatures 50-800 K. With the use of $k \cdot p$ theory, we find the non-parabolicity of the electronic band structure, and describe how to include it in the Tanguy model. Herewith we achieve a better agreement between the theory and the experimental data.

[1] Schweizer et. al., Phys. Rev. Lett. **51**, (1983)
[2] Tanguy, Phys. Rev. B **60**, (1999)

DS 21.8 Fri 11:45 REC/C213

A Novel Characterization Tool for Optical Coatings and Thin Films — •Fabian Felixberger[1,2], Ayesha Khan[1,3], Jonathan Noé[1], Michael Förg[1], Manuel Nutz[1], Simone Strohmair[1], Ines Amersdorffer[1,3], David Hunger[3], Theodor Hänsch[2], and Thomas Hümmer[1] — [1]Qlibri GmbH, Munich — [2]Ludwig Maximilian University of Munich — [3]Karlsruhe Institute of Technology

Thin films and nanostructured surfaces play a crucial role in modern science and technology, with their applications ranging from optical components to biosensors. Their precise characterization is therefore essential for understanding and optimizing their function.

We show that inserting such materials in an optical resonator [1] offers a platform which allows the investigation of minimal amounts of scattering and absorption. In addition, it can be utilised for the detection of defects, deviations from surface flatness and local changes of the refractive index.

By raster-scanning the sample, we obtain spatially resolved maps that allow us to distinguish between point-like defects and extended surface features.

Our results prove that we have developed a versatile and open-access tool for non-destructive and quantitative analysis of optical coatings and thin films, suitable for a wide range of materials.

[1] T. Hümmer et al., Nat Commun. 7, 12155 (2016)

DS 21.9 Fri 12:00 REC/C213

Measuring sub-nanometer oscillations of a thin gold film by a combination of ultrafast imaging ellipsometry and interferometry — •Markus Olbrich[1,2], Theo Pflug[1,3], Andy Engel[1], Andrés Lasagni[2,4], and Alexander Horn[1] — [1]Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany — [2]Institut für Fertigungstechnik, Technische Universität Dresden, George-Bähr-Str. 3c, 01069 Dresden, Germany — [3]Carl Zeiss SMT GmbH, Carl-Zeiss-Promenade 10, 07745 Jena, Germany — [4]Fraunhofer-Institut für Werkstoff- und Strahltechnik IWS, Winterbergstr. 28, 01277 Dresden, Germany

Measuring the transient dielectric function of laser-excited surfaces by ultrafast optical metrology is crucial for understanding fundamental processes such as the absorption of laser radiation, the dynamics of the electron-phonon non-equilibrium, or material ablation. Thereby, the measured transient dielectric function always represents the sum of changes in the optical properties and topography. To distinguish between these two contributions, a combination of ultrafast ellipsometry and ultrafast interferometry enables solving this problem. To demonstrate the advantage of the combination of both methods, the transient changes in the dielectric function and the surface topography in terms of periodic oscillations due to the induced shock and rarefaction waves are exemplarily demonstrated for an excited thin gold film upon single-pulsed irradiation with ultrafast laser radiation ($\lambda = 800\,\mathrm{nm}$, $\tau_H = 40\,\mathrm{fs}$) at a fluence of 50 % of the ablation threshold.

DS 21.10 Fri 12:15 REC/C213

Long-term studies of the defect types in tritiated graphene using Raman microscopy — •Genrich Zeller[1], Magnus Schlösser[1], and Helmut H. Telle[2] — [1]KIT-IAP, Karlsruhe, Germany — [2]UAM, Madrid, Spain

Tritium loading of graphene and graphene-like materials is of interest, e.g., in astroparticle physics, where such materials are proposed as sources and targets for neutrino experiments like KATRIN or PTOLEMY, or in hydrogen-isotope separation membranes for nuclear fusion. Although hydrogenation of graphene is well established, the radioactive nature of tritium introduces additional experimental challenges and open questions.

Only in recent years has tritiation of graphene been demonstrated using self-radiolysis of tritium. In that initial proof-of-principle study, we found that tritium exposure not only led to the adsorption of atomic tritium but also to the creation of vacancy defects. A key component of the analysis of tritiated graphene is high-resolution Raman spectroscopy, which allows us to measure defect densities and to determine the nature of the defects. In this work, we follow up on our initial studies, and we observe the evolution of defect types during three years of storage under ambient conditions. We find that graphene adsorption sites become strongly depleted, evidenced by the recovery of the characteristic 2D band and an overall decrease in defect density as tracked by the D/G band ratio. The magnitude of this depletion substantially exceeds the annual reduction expected from tritium β-decay alone, indicating additional removal pathways besides radioactive decay.