Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls SCH A 315 and SCH A 316; Poster P3)

Gaede Prize Talk

PRV II	Wed	13:15–13:45	HSZ 01	**Towards chemical and optical band structure engineering in molecular-based heterostructures** — •Benjamin Stadtmueller

Invited Talks

DS 5.1	Tue	9:30–10:00	SCH A 316	***Operando* infrared studies of confined water and protons in MXene** — •Mailis Lounasvuori
DS 9.1	Wed	9:30–10:00	SCH A 316	**Flüssigphasen-Elektrochemie im Ultrahochvakuum unter XPS-Kontrolle** — •Frank Endres
DS 13.1	Thu	9:30–10:00	SCH A 316	**Towards Catalytic Applications of Infrared Laser Polarimetry** — •Andreas Furchner, Karsten Hinrichs
DS 15.1	Thu	11:15–11:45	SCH A 316	**In-Situ Optical Investigation of Electrochemically Induced Conformational Changes at Solid Liquid Interfaces: A Source of new Electronic States** — •Christoph Cobet
DS 17.1	Thu	16:15–16:45	SCH A 316	**In-situ optical spectroscopy on electrochemical interfaces: From OER electrocatalysts to "smart" electro-switchable interfaces** — •Martin Rabe
DS 17.2	Thu	16:45–17:15	SCH A 316	**The physics of low symmetry semiconductors: Gallium oxide for the future of green energy as example** — •Mathias Schubert
DS 17.3	Thu	17:15–17:45	SCH A 316	**Spectroscopic ellipsometry studies of optical constants in highly excited semiconductors** — •Stefan Zollner

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers
SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Ultrafast Excitation Pathways of Quantum Materials (SYUE)

See SYUE for the full program of the symposium.

SYUE 1.1	Wed	9:30–10:00	HSZ 01	**Dynamics and control in quantum materials using multi-terahertz spectroscopy** — •Richard Averitt
SYUE 1.2	Wed	10:00–10:30	HSZ 01	**Accessing the nonthermal phonon populations in 2D materials with femtosecond electron diffuse scattering** — •Hélène Seiler
SYUE 1.3	Wed	10:30–11:00	HSZ 01	**Exciting potentials – Exploring the realms of ultrafast phase transitions** — •Laurenz Rettig
SYUE 1.4	Wed	11:15–11:45	HSZ 01	**Sub-cycle multidimensional spectroscopy of strongly correlated materials** — •Olga Smirnova
SYUE 1.5	Wed	11:45–12:15	HSZ 01	**Witnessing many-body entanglement in light-driven quantum materials** — •Matteo Mitrano
SYUE 1.6	Wed	12:15–12:45	HSZ 01	**Optical responses of photoexcited materials: from parametric amplification to photoinduced superconductivity** — •Eugene Demler

Invited Talks of the joint Symposium Physics of van der Waals 2D Heterostructures (SYHS)

See SYHS for the full program of the symposium.

SYHS 1.1	Fri	9:30–10:00	HSZ 01	**Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures** — •Steven G. Louie
SYHS 1.2	Fri	10:00–10:30	HSZ 01	**Interaction induced magnetism in 2D semiconductor moiré superlattices** — •Xiaodong Xu
SYHS 1.3	Fri	10:30–11:00	HSZ 01	**Ions in tight places: intercalation and transport of ions in van der Waals heterostructures** — •Irina Grigorieva
SYHS 1.4	Fri	11:15–11:45	HSZ 01	**Spin-orbit proximity in van der Waals heterostructures** — •Felix Casanova
SYHS 1.5	Fri	11:45–12:15	HSZ 01	**Plethora of many-body ground states in magic angle twisted bilayer graphene** — •Dmitri Efetov

Sessions

DS 1.1–1.6	Mon	9:30–11:00	SCH A 316	**2D Materials and their Heterostructures I: Graphene**
DS 2.1–2.5	Mon	11:30–12:45	SCH A 316	**2D Materials and their Heterostructures II: h-BN and WSe_2**
DS 3.1–3.5	Mon	11:30–12:45	SCH A 315	**Organic Thin Films, Organic-Inorganic Interfaces (joint session DS/CPP)**
DS 4.1–4.6	Mon	15:30–17:00	SCH A 316	**Thin Film Properties I**
DS 5.1–5.4	Tue	9:30–10:45	SCH A 316	**2D Materials and their Heterostructures III**
DS 6.1–6.4	Tue	10:00–11:00	SCH A 315	**Thin Film Properties II (joint session DS/KFM)**
DS 7.1–7.5	Tue	11:15–12:30	SCH A 316	**2D Materials and their Heterostructures IV**
DS 8.1–8.5	Tue	11:30–12:45	SCH A 315	**Thin Film Properties III**
DS 9.1–9.3	Wed	9:30–10:30	SCH A 316	**Layer Properties I**
DS 10.1–10.5	Wed	11:00–12:15	SCH A 316	**Layer Properties II**
DS 11.1–11.5	Wed	11:00–12:15	SCH A 315	**Thin Film Application**
DS 12.1–12.57	Wed	17:00–19:00	P3	**Poster**
DS 13.1–13.5	Thu	9:30–11:00	SCH A 316	**Optical Analysis of Thin Films I**
DS 14.1–14.7	Thu	9:30–11:15	SCH A 315	**Thin Oxides and Oxide Layers**
DS 15.1–15.5	Thu	11:15–12:45	SCH A 316	**Optical Analysis of Thin Films II**
DS 16.1–16.6	Thu	11:30–13:00	SCH A 315	**Thermoelectric and Phase Change Materials; Layer Deposition**
DS 17.1–17.3	Thu	16:15–17:45	SCH A 316	**Optical Analysis of Thin Films III**
DS 18	Thu	18:00–19:00	SCH A 315	**Members' Assembly**

Members' Assembly of the Thin Films Division

Thursday 18:00–19:00 SCH A 316

DS 1: 2D Materials and their Heterostructures I: Graphene

Time: Monday 9:30–11:00 Location: SCH A 316

DS 1.1 Mon 9:30 SCH A 316

Atomistic and network models for graphene based macromaterials: role of intercalation, defects and dopants — •Florian Fuchs[1,2] and Jörg Schuster[1,2] — [1]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

The excellent properties of graphene can be utilized in macroscopic conductor materials if the individual flakes are decoupled from each other, for example by misalignment of the lattices or by intercalation. Such materials are promising candidates to replace metals for numerous electrical conductor applications [1].

We show the results of a network model [2,3] which relates the structural arrangement and the properties of the individual graphene flakes to the macroscopically observed electrical conductivity. By this model we assess the properties of the macromaterial as a function of relevant parameters such as flake size, packing density, the graphene flake conductivity, and the interlayer conductance.

On the flake-level, intercalation, doping, and defect healing control the conductivity of the graphene-based macromaterial. We performed density functional theory calculations of these processes. In our presentation we discuss the impact on the material quality by focussing on the in-plane and the out-of-plane conductivity.

[1] J. Schuster et al., Nano Express 1, 020035 (2020)
[2] J. Schuster et al., ACS Appl. Mater. Interfaces 10, 43008 (2018)
[3] J. Schuster et al., Comp. Mat. Science 161 , 364 (2019)

DS 1.2 Mon 9:45 SCH A 316

Post-processing on graphene field-effect transistors by critical point drying — •Hamid Reza Rasouli[1], David Kaiser[1], Christof Neumann[1], Martha Frey[1], Ghazaleh Eshaghi[1], Thomas Weimann[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany

We report on a critical point drying (CPD) technique with supercritical carbon dioxide (S-CO2) as a post-processing step to enhance electrical performance of graphene field-effect transistors (GFETs). This technique is promising for integration into the industrial clean rooms environment and demonstrates high potential not only for GFETs but also for other electronic, photonic and optoelectronic devices based on 2D materials.

DS 1.3 Mon 10:00 SCH A 316

Intercalation of indenene in SiC/graphene interface — •Cedric Schmitt[1,2], Jonas Erhardt[1,2], Tien-Lin Lee[3], Timur Kim[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]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK

In the search for new quantum materials, ultrathin metals are highly interesting as they push bulk properties to the 2D limit and foster novel quantum effects. Unfortunately, unprotected metals are prone to oxidation in air, making them useless for transport devices. Here, we report about a capping method for 2D materials via metal intercalation. In this process an atomic metal monolayer is sandwiched between a SiC substrate and a graphene buffer layer, thus forming freestanding graphene, which protects the intercalated layer against oxidation. Previous intercalation studies focused mainly identifying stable allotropes but lack a detailed investigation of metal coverage and oxidation. Here, we study the intercalation of indenene, a monolayer of indium, which is a novel quantum material [1]. First experiments indicate the indenene layer to remain intact upon air exposure, indeed pointing to an effective protective function of the overlayer graphene. Furthermore, we observe an enlarged In-Si bond distance, which is expected to have a larger non-trivial energy gap.

[1] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)

DS 1.4 Mon 10:15 SCH A 316

Ultrafast photo-thermoelectric currents in graphene — •Xiaoyi Zhou, Nina Pettinger, Johannes Gröbmeyer, Philipp Zimmermann, and Alexander Holleitner — Walter Schottky Institut and Physics Department, Technische Universität München, Germany

Graphene as an optoelectronic material has attracted significant attention due to its interesting properties such as fast charge carrier relaxation rates, broadband optical absorption and high carrier mobilities. We apply an ultrafast on-chip pump-probe photocurrent spectroscopy to demonstrate an immediate thermoelectric photocurrent after a femtosecond laser pulse. We demonstrate that gate-tunable graphene junctions can be integrated into THz-circuits, paving the way for graphene-based ultrafast photodetectors and switches.

DS 1.5 Mon 10:30 SCH A 316

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

We investigate the proximity-induced spin-orbit coupling in twisted heterostructures of graphene/transition-metal dichalcogenides (MoS_2, WS_2, $MoSe_2$, and WSe_2) as well as graphene/topological insulators (Bi_2Se_3 and Bi_2Te_3) from first principles. We establish that, regardless of the twist angle, the band offsets between the Dirac point and the substrate bands vary linearly with the strain, which is necessary for defining commensurate supercells. This relation allows to identify the apparent zero-strain band offsets and find a compensating transverse electric field correcting for the strain. The resulting corrected band structure is then fitted around the Dirac point to an established spin-orbit Hamiltonian, yielding the twist angle dependencies of the spin-orbit couplings. While for most structures a mix of Rashba and valley-Zeeman spin-orbit coupling is present, we also witness the emergence of Kane-Mele spin-orbit coupling in graphene/topological insulator structures at 30° twist angle. This work was funded by the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG), SFB 1277, SPP 2244 and by the European Union Horizon 2020 Research and Innovation Program under contract number 881603 (Graphene Flagship). M.G. acknowledges VEGA 1/0105/20.

DS 1.6 Mon 10:45 SCH A 316

Mobile trions in two-dimensional hybrid perovskites — Jonas David Ziegler[1], Yeongsu Cho[2], •Sophia Terres[1], Matan Menahem[3], Omer Yaffe[3], Takashi Taniguchi[4], Kenji Watanabe[4], Timothy C. Berkelbach[2], and Alexey Chernikov[1] — [1]TU Dresden, Dresden, Deutschland — [2]Columbia University, New York, USA — [3]Weizmann Institute of Science, Rehovot, Israel — [4]National Institute for Materials Science, Tsukuba, Japan

Two-dimensional hybrid perovskites represent natural quantum well systems composed of alternating organic and inorganic molecular layers. They combine an efficient coupling of electrons to a soft lattice with strong Coulomb interactions between the charge carriers. The latter leads to the formation of tightly bound excitons that determine the optical response of this class of materials. The interaction between excitons and free charge carriers, however, remains difficult to access in halide perovskites due to persistent challenges to introduce doping.

Here, we report experimental realization of electrically tunable, ultrathin two-dimensional perovskites, by combining them with hBN and multilayer graphene in field-effect transistor geometries. We demonstrate the formation of both negatively and positively charged exciton-electron complexes, known as trions with binding energies up to 46 meV. These values are a direct consequence of strong Coulomb interaction and scale with exciton binding energies, as demonstrated by theoretical calculations. The trions exhibit finite oscillator strength in absorption-like response, are localized at cryogenic temperatures, and exhibit thermally activated diffusion at 50 K.

DS 2: 2D Materials and their Heterostructures II: h-BN and WSe_2

Time: Monday 11:30–12:45 Location: SCH A 316

DS 2.1 Mon 11:30 SCH A 316

Engineering of exciton g-factors in van der Waals structures — •Tomasz Woźniak[1], Paulo Faria Junior[2], Andrey Chaves[3], Umm-e-hani Asghar[4], and Agnieszka Kuc[5] — [1]Wrocław University of Science and Technology, Poland — [2]Universitaet Regensburg, Germany — [3]Universidade Federal do Ceará, Brazil — [4]Jacobs Universitaet Bremen, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany

We develop a fully ab-initio based calculation scheme for excitonic g-factors, which describe their energy dependence on external magnetic field, and apply it to 1L TMDs and $MoSe_2/WSe_2$ heterobilayers, obtaining excellent agreement with experiments [1]. We identify a series of magneto-PL peaks in 1L WS_2 based on the calculated g-factors of excitons, trions and biexcitons, as well as phonon replicas of the dark trion [2]. We explain the reduction of g-factor measured in $MoSe_2/WS_2$ by the spatial confinement of the intralayer moiré exciton [3]. We find a significant strain dependence of excitonic g-factors and dipole strengths in 1L TMDs. It allows to explain the strain-induced hybridization of direct and indirect excitons in WS_2 [4,5]. We investigate a new class of hexagonal materials with formula MSi_2Z_4 (M: Mo, W; Z: N, P, As, Sb), which are isosymmetric to 1L TMDs. We find a new set of circularly polarized excitonic transitions with high binding energies and large positive g-factors [6].

[1] Phys. Rev. B 101, 235408 (2020) [2] Nano Lett. 21, 2519 (2021) [3] Nano Lett. 21, 8641 (2022) [4] Phys. Rev. Lett. 129, 067402 (2022) [5] New J. Phys. 24, 083004 (2022) [6] arXiv:2210.10679 (2022)

DS 2.2 Mon 11:45 SCH A 316

Phase-locked photon-electron interaction without a laser applied to 2D Materials — •Nahid Talebi[1], Masoud Taleb[1], Mario Hentschel[2], Kai Rossnagel[1], and Harald Giessen[2] — [1]Institute for Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Ultrafast electron-photon spectroscopy in electron microscopes commonly requires ultrafast laser setups. Photoemission from an engineered electron source is used to generate pulsed electrons, interacting with a sample that is excited by the ultrafast laser pulse at a specified time delay. Here, we present an inverse approach based on cathodoluminescence spectroscopy to introduce internal radiation sources in an electron microscope. Our method is based on a sequential interaction of the electron beam with an electron-driven photon source (EDPHS) and the investigated sample. An electron-driven photon source in an electron microscope generates phase-locked photons that are mutually coherent with the near-field distribution of the swift electron. We demonstrate the mutual coherence between the radiations from the EDPHS and the sample by performing interferometry with a combined system of an EDPHS and a WSe2 flake. Our method has the advantage of being simple, compact and operating with continuous electron beams. It will open the door to local electron-photon correlation spectroscopy of quantum materials, single photon systems, and coherent exciton-polaritonic samples with nanometric resolution.

DS 2.3 Mon 12:00 SCH A 316

Phase-locked photon-electron interaction without a laser applied to 2D Materials — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany

Ultrafast electron-photon spectroscopy in electron microscopes commonly requires ultrafast laser setups. Photoemission from an engineered electron source is used to generate pulsed electrons, interacting with a sample that is excited by the ultrafast laser pulse at a specified time delay. Thus, developing an ultrafast electron microscope demands the exploitation of extrinsic laser excitations and complex synchronization schemes. Here, we present an inverse approach based on cathodoluminescence spectroscopy to introduce internal radiation sources in an electron microscope. Our method is based on a sequential interaction of the electron beam with an electron-driven photon source (EDPHS) and the investigated sample. An electron-driven photon source in an electron microscope generates phase-locked photons that are mutually coherent with the near-field distribution of the swift electron. We demonstrate the mutual coherence between the radiations from the EDPHS and the sample by performing interferometry with a combined system of an EDPHS and a WSe2 flake. Our method has the advantage of being simple, compact and operating with continuous electron beams. It will open the door to local electron-photon correlation spectroscopy of quantum materials, single photon systems, and coherent exciton-polaritonic samples with nanometric resolution.

DS 2.4 Mon 12:15 SCH A 316

Mobile interlayer excitons at the Mott transition in Moiré-free heterostructures — •Edith Wietek[1], Mikhail M. Glazov[2], Matthias Florian[3], Takashi Taniguchi[4], Kenji Watanabe[4], Alexander Steinhoff[5], and Alexey Chernikov[1] — [1]Technische Universität Dresden — [2]Sankt Petersburg — [3]University of Michigan — [4]NIMS, Ibaraki — [5]Universität Bremen

Vertically stacked heterostructures of transition metal dichalcogenides present an exciting platform to study electronic and excitonic many-particle states. In this study we investigate propagation of excitons in these systems from low to very high densities to disentangle the effects of dipolar excitons from those stemming from moiré effects. We take advantage of hBN-encapsulated WSe2/MoSe2 heterostructures studied in the moiré-free limit of large, atomically reconstructed domains. Using ultrafast microscopy, we show that the interlayer excitons propagate freely even at cryogenic temperatures and low densities. At elevated exciton densities, we demonstrate that in addition to broadly assumed exciton-exciton repulsion, the non-linear increase of the diffusion coefficient also originates from efficient exciton-exciton annihilation. Remarkably, at the exciton ionization threshold of the Mott transition and beyond, we reveal a highly unusual regime of negative effective diffusion that persist for many 100's of ps after the excitation. This observation presents a particularly interesting case of non-equilibrium phenomena in composite many-particle systems, highlighting the rich physics of optical excitations in van der Waals heterostructures.

DS 2.5 Mon 12:30 SCH A 316

Atomic structures of single photon emitters in hexagonal boron nitride — •Tjorben Matthes[1], Anand Kumar[1], Chanaprom Cholsuk[1], and Tobias Vogl[1,2] — [1]Institute of Applied Physics, Friedrich-Schiller-University Jena, Albert-Einstein-Straße 15, 07745 Jena — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Albert-Einstein-Str. 7, 07745 Jena

Single photon emitters in solid-state crystals have received a lot of attention as building blocks for numerous quantum technology applications. Fluorescent defects in hexagonal boron nitride (hBN) stand out due to their high luminosity and robust operation at room temperature. The fabrication of identical emitters at pre-defined sites is still challenging, which hampers the integration of these defects in optical systems and electro-optical devices. Additionally, the atomic structure of many defects remain unclear or are subject to ambiguous guess-work. Here, we show an analysis on the atomic structures of defects we created by electron beam irradiation using a standard scanning electron microscope with deep sub-micron lateral precision. The emitters are created with a high yield and a reproducible spectrum peaking at 575 nm. We also present results on correlating crystal structure properties and polarization dynamics. Our results indicate that these emitters that all emitters are identical, which is a crucial advantage for the realization of quantum integrated devices, as well as for the identification of these fluorescent defects.

DS 3: Organic Thin Films, Organic-Inorganic Interfaces (joint session DS/CPP)

Time: Monday 11:30–12:45 Location: SCH A 315

DS 3.1 Mon 11:30 SCH A 315

Thickness dependency of the critical dose for beam-sensitive two-dimensional polymers — •David Mücke[1], Ute Kaiser[1], and Haoyuan Qi[1,2] — [1]Central Facility of Material Science Electron Microscopy, Universität Ulm, 89081 Ulm, Germany — [2]Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

For organic materials the achievable resolution in a TEM is limited by their resilience against electron irradiation. Due to that, increasing the critical dose of these sensitive materials is of highest importance. For layer stacked materials, where the thickness is easily controllable, the thickness dependency of the critical dose is a key feature. Aimed at gathering a better understanding of this effect, in our study this dependency was examined in more detail. To achieve this, the critical dose of a triazine-based 2D polymer[1] was measured for a wide thickness range. The polymer samples, obtained by mechanical exfoliation, ranged from 15 nm to 85 nm thickness. To obtain the critical dose of the polymer, sequences of electron diffraction patterns with a dose of only 0.5 e^-/A^2 where obtained. The measurements revealed, that the critical dose for amorphization of this polymer is only 1-2 e^-/A^2, independent of sample thickness.

References
1. F. Hu, et al. J. Am. Chem. Soc. 143, 5636-5642 (2021).

DS 3.2 Mon 11:45 SCH A 315

Determining Anisotropic Effects in Strongly Coupled Metal Organic Hybrid Structures — •Maximilian Rödel[1], Jinhong Kim[2], Matthias Stolte[2], Luca Nils Philipp[3], Matthias Lehmann[2], Frank Würthner[2], Roland Mitric[3], and Jens Pflaum[1,4] — [1]Experimental Physics VI, University of Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg — [3]Institut für Physikalische und Theoretische Chemie, University of Würzburg — [4]Bavarian Center for Applied Energy Research, 97074 Würzburg

Coupling phenomena in metal organic hybrid structures enable unique possibilities to tune the properties of opto-electronic devices. Furthermore, the strong coupling between surface plasmons and excitons in organic semiconductors leads to novel hybrid states, which are termed plexcitons[1]. By means of a Kretschmann Set Up we investigate these plexcitonic states in oriented liquid crystalline perylene bisimide (PBI) thin films deposited via off-centered spin coating on gold surfaces which exhibiting J-type coupling [2]. The Alignment of the hydrogen-bonded PBI molecules and, thus, their transition dipoles results in long-range ordered films with a pronounced spatially anisotropy of structural and optical characteristics. These new states show a characteristic coupling strength of ≈27 meV. Understanding this directional correlation between molecular order and optical properties will enable new device concepts utilizing the presented opto-electronic directionality.

[1] Maximilian Rödel et al. J. Phys. Chem. C 2022, 126(8), 4163-4171
[2] Stefanie Herbst et al. Nat. Commun. 2018, 9(1), 2646-2654.

DS 3.3 Mon 12:00 SCH A 315

Long-term degradation in Blatter radical derivative thin films — •Ewa Nowik-Boltyk, Tobias Junghöfer, and Maria Benedetta Casu — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, D-72076 Tübingen,GERMANY

Materials with a radical site are strong candidates for ground-breaking applications from energy storage to quantum computing. In this framework, Blatter radical derivatives are very attractive due to their chemical stability. We focus on the latest insights regarding the fundamental mechanisms of radical thin film long-term degradation, by comparing two Blatter radical derivatives, using X-ray-based techniques, such as photoelectron spectroscopy and absorption spectroscopy. Our findings indicate that air exposure affects the chemical and magnetic properties of the thin films.

DS 3.4 Mon 12:15 SCH A 315

Controlled Thermal Deposition of Organic Diradicals — •Tobias Junghöfer and Maria Benedetta Casu — Institut für Physikalische und Theoretische Chemie, Eberhard Karls Universität Tübingen, Germany

Using X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) we demonstrate that it is possible to evaporate diradicals in a controlled environment obtaining thin films in which the diradical character is preserved. However, evaporation represents a challenge. The presence of two radical sites makes the molecules more reactive also in the case of very stable single radicals. We have explored the parameters that play a role in this phenomenon. We found that the higher the formation energies of the crystal, the more difficult is the evaporation of intact radicals. Large delocalization of the unpaired electrons helps the diradical to stand evaporation. The evaporation of different diradicals can be successfully addressed considering our findings.

DS 3.5 Mon 12:30 SCH A 315

Interaction of cyanoacrylate thin films with copper (oxide) in different processing atmospheres — •Philipp Moritz[1], Oliver Höfft[2], Lienhard Wegewitz[1], and Wolfgang Maus-Friedrichs[1] — [1]Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastrasse 2, 38678 Clausthal-Zellerfeld — [2]Institute of Electrochemistry, Clausthal University of Technology, Arnold-Sommerfeld-Strasse 6, 38678 Clausthal-Zellerfeld

The adhesive class of fast-curing cyanoacrylates plays an increasingly important role, especially in hybrid composites. However, the adhesion mechanism at the interface to the metal (oxide) substrates is not sufficiently understood.

To study the interactions, cyanoacrylate films of a few nm thickness are spin-coated onto metallic copper and copper oxide in (i) a normal air atmosphere and in (ii) an oxygen-free environment (O_2 partial pressure $< 10^{-20}$ mbar). The natively oxidized copper is deoxidized with a dielectric barrier discharge (DBD plasma) directly before the coating process.

Spectroscopic and microscopic methods are used to understand the underlying molecular interactions at the interface between cyanoacrylate and copper (oxide). The formation of hydrogen bonds as well as an ionic interaction can be observed. In addition, an influence of the oxide layer and the effects of the surrounding atmosphere can be seen.

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DS 4: Thin Film Properties I

Time: Monday 15:30–17:00 Location: SCH A 316

DS 4.1 Mon 15:30 SCH A 316

Ultrafast laser induced structural motion in crystalline and amorphous gold — •Othmane Benhayoun[1], Emiliano Principi[3], Bernd Bauerhenne[1], Dmitry S. Ivanov[2], and Martin E. Garcia[1] — [1]University of Kassel, Theoretical physics II, Kassel, Germany — [2]Moscow, Russia — [3]Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

A recent Ultrafast Electron Diffraction (UED) experiment showed a time-dependent nonuniform compression and expansion of a monocrystalline gold foil. This led to the time modulation of the Au Bragg peaks in both height and width. The same effect is however not observed in polycrystalline gold. We thus perform Molecular Dynamics - Two Temperature Model (MD-TTM) simulations aiming to understand the results of the experiment. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics.

DS 4.2 Mon 15:45 SCH A 316

Co-electrodeposition of compositionally complex Co-Cr-Fe-Mo-Ni alloy thin films — •Hongshuai Li, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

A compositionally complex Co-Cr-Fe-Mo-Ni alloy with a face-centered cubic structure was successfully obtained by electrochemical deposition using a constant current density. An aqueous electrolyte with several additives was developed to accomplish the electrodeposition of films onto Cu substrates. The characterization reveals that the deposited films are metallic with a face-centered cubic structure, including impurities incorporated during deposition. In addition, mechanical tests were performed to study adhesion and hardness by nano-scratch tests and nanoindentation. Mechanical tests show a high hardness and nonetheless microscopically ductile behavior. The electrolytes developed in this study may be a promising approach for the electrodeposition of Co-Cr-Fe-Mo-Ni compositionally complex alloy coatings.

DS 4.3 Mon 16:00 SCH A 316

Thermally controlling the length of transition and alkali metal squarate wires — •Egzona Isufi Neziri[1,2], Karl-Heinz Ernst[1,2], and Christian Wäckerlin[3,4] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]University of Zürich, 8006 Zürich, Switzerland — [3]Paul Scherrer Institute, 5232 Villigen, Switzerland — [4]EPFL, Swiss Federal Institute of Technology Lausanne, 1015 Lausanne, Switzerland

Low-dimensional metal-organic nanomaterials on surfaces can be engineered to yield promising, novel and highly customizable chemical/physical properties such as magnetism, electronic structure and catalytic properties. A variety of metal elements, including alkali, transition and even lanthanide metals have been used to direct the metal-organic assembly.

Here metal-organic structures obtained from squaric acid (H2C4O4) molecules, co-deposited with K and Ni atoms on a hot Au(111) surface, are studied by XPS and STM. We find that both K and Ni lead to the formation of condensed arrays of wires, composed of M-squarate (C4O4(2-)). Controlling the length of these wires is possible by a thermally activated process: Ni-squarate wires tend to get longer at higher temperatures while K-squarate wires get shorter.

DS 4.4 Mon 16:15 SCH A 316

Deep learning-supported in-situ HRTEM experiments on single-layer carbon — •Christopher Leist[1], Haoyuan Qi[1,2], and Ute Kaiser[1] — [1]Central Facility Materials Science Electron Microscopy, Ulm University, 89081 Ulm, Germany — [2]Faculty of Chemistry and Food Chemistry Dresden, Technische Universität Dresden, 01062 Dresden, Germany.

We perform in-situ experiments on single-layer carbon using the Cc/Cs-corrected low-voltage transmission electron microscope SALVE, resolving structure and dynamics down to the level of the single atom. These types of experiments create large amounts of data both in terms of numbers of individual images acquired and the amount of information per image. Conventional image analysis methods, e.g., handcrafted filter kernels, often require heavy user supervision and tremendous time cost, posing strong limitations on the data volume making them inconvenient for use in these experiments. Deep learning in the form of convolutional neural networks offers a reliable and effective way to handle large amounts of complex image data. Using simulated data we train a modified U-Net like neural network to identify atom positions and their structure i.e. polygons while at the same time removing contaminated areas from the evaluation in real micrographs. Thus, gaining the ability for both largescale statistical evaluation and mapping atomically-resolved the material's transformation.

DS 4.5 Mon 16:30 SCH A 316

Microstructure and mechanical properties of Ta-Al-B coatings — •Chun Hu[1], Shuyao Lin[1], Maximilian Podsednik[2], Andreas Limbeck[2], Nikola Koutná[1], and Paul H. Mayrhofer[1] — [1]Institute of Materials Science and Technology,TU Wien,Getreidemarkt 9,Vienna,A-1060,Austria — [2]Institute of Chemical Technologies and Analytics, TU Wien, A-1060 Wien, Austria

Alloying is a simple yet powerful tool to tune properties of hard coatings. Here we report stoichiometry, microstructure and hardness evolution of Al-alloyed TaB2-z coatings. Sputtering a stoichiometric TaB2 target results in sub-stoichiometric TaB1.23 with a mixed hexagonal-TaB2 (α-AlB2-type) and orthorhombic TaB structure. Co-sputtering an AlB2 target*with half the sputtering power density*increases the B content and strongly promotes the α-phase, while only little Al is incorporated (Ta0.997Al0.003B1.64). The coating shows a small grain size and the overall highest hardness. Further increasing the AlB2/TaB2 sputter ratio allows for B/Metal ratios of 1.97 and 2.29 with Al metal-fractions up to 48 at%. These coatings are single-α-phased with a smooth surface but gradually decreased hardness due to the increased AlB2-fraction. The structural evolutions are underpinned by ab initio calculations.

DS 4.6 Mon 16:45 SCH A 316

X-ray characterization of an above-RT bi-stable sublimable molecular spin-crossover Fe(II)-complex — •Yahya Shubbak[1], Miguel Gavara Edo[2], Arno Ehresmann[1], and Eugenio Coronado Mirales[2] — [1]Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, D-34132 Kassel — [2]Institute of Molecular Science (ICMol), University of València, S-46980 Paterna

Spin crossover (SCO) molecules are a promising type of material that can undergo reversible switching between low-spin (LS)- and high-spin (HS)-states upon external stimuli (heat, light, pressure, etc.)[1], making them useful for information technology, data storage, and optoelectronics[2]. However, most SCO molecules need to be cooled significantly for this transition to be observable. We have investigated the hitherto unknown electronic structure of the complex molecule bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(II) ([Fe(HB(tz)3)2])[3] capable of above-RT transition by XPS and XAS measurements, since the distinct electronic structure in both spin-states unmistakably prove the transition between them. [1]P. Gütlich and H. A. Goodwin. Spin Crossover in Transition Metal Compounds I. Springer Berlin Heidelberg, May 2004. 356 pp. [2]E. P. Geest et al., Contactless Spin Switch Sensing by Chemo-Electric Gating of graphene. In: Advanced Materials (2020), p. 1903575. [3]S. Rat et al., Solvatomorphism and structural-spin crossover property relationship in bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(ii). In: CrystEngComm 19.24 (2017).

DS 5: 2D Materials and their Heterostructures III

Time: Tuesday 9:30–10:45 Location: SCH A 316

Invited Talk DS 5.1 Tue 9:30 SCH A 316

***Operando* infrared studies of confined water and protons in MXene** — •Mailis Lounasvuori — Helmholtz-Zentrum Berlin, Berlin, Germany

MXenes are a large family of 2-dimensional transition metal carbides, nitrides and carbonitrides with excellent potential for energy storage applications. Due to hydrophilic surfaces and weak attractive forces between the negatively charged layers, MXenes can retain significant amounts of water between the layers, and they can be intercalated with a variety of cations and molecules. Here, I will present our recent research efforts to apply *operando* infrared spectroscopy to probe the vibrational dynamics of water confined between Ti_3C_2 MXene sheets during electrochemical charging and discharging. Data for both lithium- and proton-containing electrolytes will be presented. Potential-dependent, reversible changes in the O-H stretching modes of confined water are observed that are specific to the cation. In acidic electrolyte, we observe a unique signature of confined hydrated protons which is not seen in the bulk.

DS 5.2 Tue 10:00 SCH A 316

Contact Printed Micro Circuit Boards - A Novel Platform for the Defect Free Integration of 2D Materials — •Christian N. Saggau[1], Sanaz Shokri[1,2], Yejin Lee[1,2], Mickey Martini[1,2], Tommaso Confalone[1], Genda Gu[3], Valentina Brosco[4], Domenico Montemurro[5], Valerii M. Vinokur[6], Kornelius Nielsch[1,2,7], and Nicola Poccia[1] — [1]Leibnitz Institute for Solid State and Materials Science Dresden, Dresden, Germany — [2]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany — [3]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, USA — [4]Italian National Research Council, Institute for Complex Systems, Rome, Italy — [5]Department of Physics, University of Naples Federico II, Naples, Italy — [6]Terra Quantum AG, St. Gallen, Switzerland — [7]Institute of Materials Science, Technische Universität Dresden, Dresden, Germany

The 2D cuprate superconductor BSCCO, promises upon integration with CMOS electronics, on-chip high temperature superconducting single photon detectors or quantum interference device (SQUID). Unfortunately, its properties degrade quickly if exposed to elevated temperatures, solvents, oxygen or water. Here we present Hall devices with a record thin film Tc of 91 K, which is identical to the bulk value of the crystal. Electrical contacts were established through transfer-printable circuits embedded in SiNx nanomembranes. The membrane incapsulates the material shielding it from the environment, while via contacts are used to form the electrical contacts.

DS 5.3 Tue 10:15 SCH A 316

Probing magnetic ordering in air stable iron-rich van der Waals minerals — •Muhammad Zubair Khan[1], Apoorva Sharma[2], Sergio Valencia[3], Florian Kronast[3], Oleg E. Peil[4], Georgeta Salvan[2], Christian Teichert[1], and Aleksandar Matković[1] — [1]Institute of Physics, Montanuniversität Leoben, Austria. — [2]Institute of Semiconductor Physics, Technische Universität Chemnitz, Germany. — [3]Department of Spin and Topology in Quantum Materials, Helmholtz-Zentrum Berlin, Germany. — [4]Materials Center Leoben, Austria.

We demonstrate magnetic ordering in Fe-rich two-dimensional (2D) phyllosilicates: annite, minnesotaite, and biotite. These van der Waals (vdW) minerals, incorporate local moment baring iron (Fe) ions via magnesium (Mg) substitution. The phyllosilicate capping silicate/aluminate tetrahedral groups make monolayers air stable. Superconducting quantum interference device vibrating sample magnetometry (SQUID-VSM) was used probe long-range magnetic ordering in bulk. In-field magnetic force microscopy (MFM) confirmed the local magnetic moment at room temperature, present down to monolayers. X-ray photoelectron spectroscopy (XPS) were used to observe the Fe oxidation state and to establish a correlation with magnetic ordering. Further, magnetic ordering in thin flakes was probed via X-ray magnetic circular dichroism. Our study of Fe-baring vdW minerals may drive the development for controllable synthesis of novel 2D magnetic insulators.

DS 5.4 Tue 10:30 SCH A 316

Anisotropic Spontaneous Magnetostriction in $Fe_{3-x}GeTe_2$ — •Reinhard K. Kremer and Eva Brücher — MPI for Solid State Research, Stuttgart, Germany

By determining the lattice parameters as a function of temperature of the hexagonal van der Waals ferromagnet $Fe_{2.93(2)}Ge_{1.02(3)}Te_2$ we detect a spontaneous negative in-plane magnetostriction occuring below the Curie temperature. The spontaneous magnetostriction follows the square of the spontaneous magnetization and leads to an expansion of the hexagonal layers, and is clearly seen for the in-plane lattice parameter a, but less well pronounced perpendicular to the planes along c. Extrapolating to $T \to 0$ K we obtain a saturation spontaneous magnetostriction of $\lambda_{sp,a}(T \to 0)$ = -214(6) $\times 10^{-6}$ and a volume magnetotriction $\lambda_{sp,vol}(T \to 0) \approx -450 \times 10^{-6}$, indicating that the spontaneous magnetostriction along c is very small. The linear thermal expansion coefficients at 295 K of $Fe_{2.93(2)}Ge_{1.02(3)}Te_2$ amount to $13.9(1)\times10^{-6}$ K^{-1} and to $23.22(15)\times10^{-6}$ K^{-1} for the in-plane and out of plane direction, respectively, indicating in a linear volume thermal expansion coefficient of $51.0(2)\times10^{-6}$.

DS 6: Thin Film Properties II (joint session DS/KFM)

Time: Tuesday 10:00–11:00 Location: SCH A 315

DS 6.1 Tue 10:00 SCH A 315

Defect nanostructure and its impact on magnetism of α-Cr_2O_3 thin films — •Ihor Veremchuk[1], Oskar Liedke[1], Pavlo Makushko[1], Tobias Kosub[1], Natascha Hedrich[2], Oleksandr Pylypovskyi[1], Fabian Ganss[1], Maik Butterling[1], René Hübner[1], Eric Hirschmann[1], Ahmed Attallah[1], Andreas Wagner[1], Kai Wagner[2], Brendan Shields[2], Patrick Maletinsky[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Department of Physics University of Basel, Switzerland

Thin films of the magnetoelectric insulator Cr_2O_3 are technologically relevant for energy-efficient magnetic memory devices controlled by electric fields. We experimentally investigated the defect nanostructure of 250-nm-thick Cr_2O_3 thin films prepared under different conditions on single crystals of Al_2O_3 (0001) and correlate it with the integral and local magnetic properties of the samples. Positron annihilation spectroscopy reveals that the Cr_2O_3 thin films are characterized by the presence of complex defects at grain boundaries, formed by groups of monovacancies, coexisting with monovacancies and dislocations. The defect nanostructure strongly affects the magnitude of the electrical readout. Furthermore, the presence of larger defects like grain boundaries has a strong influence on the pinning of magnetic domain walls in thin films. We show that the Néel temperature is hardly affected by the formed defects in a broad range of deposition parameters.

DS 6.2 Tue 10:15 SCH A 315

Dynamics of phase transition in Lead-free Ferroelectric thin films — •Mallika Khosla[1], Jutta Schwarzkopf[1], Daniel Schmidt[2], Daniel Hensel[1], and Peter Gaal[1,2] — [1]Leibniz-Institut für Kristallzüchtung, Berlin,Germany — [2]Tailored x-ray products, Hamburg,Germany

In this contribution, we monitor the dynamics of the phase transition in Potassium Sodium Niobate (KNaxNb1-xO3) by taking snapshots of the structure after optical excitation using pulsed synchrotron radiation in a pump-probe scheme. Our sample is a 50 nm KNaxNb1-x O3 film grown on 20 nm thin SrRuO3 on TbScO3 substrate. The low-temperature phase displays a hierarchical order of domains and superdomains on sub-100 nm and on few um length scales, respectively. First, we show that laser heating with 7 ns pulses has a similar effect locally in terms of structural rearrangement as static heating of the

whole sample volume. However, in our localized excitation the transient phase transition required to transform a similar volume fraction of the sample in the high temperature phase is about 5 times higher compared to static heating. Comparison with finite-element simulations of heat-transport in our sample shows that the phase transition dynamics does not exactly follow the temperature evolution in the ferroelectric film. In addition, time-resolved diffraction imaging experiments reveal that the stability of a spatial domain morphology has a nonlinear dependence on the local laser-induced temperature. Our results indicate that it is essential to resolve both the temporal and spatial coordinate to monitor the equilibration path of such phase transition.

DS 6.3 Tue 10:30 SCH A 315

Ferroelectric thin films studied by X-ray standing waves — •Le Phuong Hoang[1], Irena Spasojevic[2], David Pesquera[2], Gustau Catalan[2], Kai Rossnagel[3,5], Jörg Zegenhagen[4], Tien-Lin Lee[4], Ivan Vartanyants[5], Andreas Scherz[1], and Giuseppe Mercurio[1] — [1]European XFEL, Schenefeld, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain — [3]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [4]Diamond Light Source, Didcot, UK — [5]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We investigated the structural properties of ferroelectric $BaTiO_3$ thin films by X-ray standing waves with the goal to determine the atomic positions within the tetragonal unit cell in samples with different strain. Our samples consist of $BaTiO_3$ thin films grown by pulsed laser deposition (with a $SrRuO_3$ bottom electrode) on three different substrates $SmScO_3$, $GdScO_3$, $DyScO_3$ providing increasing compressive strain. All the samples were characterized by X-ray reflectivity (XRR) and reciprocal space mapping (RSM). We present X-ray photoelectron spectroscopy, X-ray diffraction and X-ray standing waves data measured at the Diamond Light Source that provide Ba and Ti atomic positions within the unit cells of sample surface. In this study we show a relation between atomic positions and compressive strain of ferroelectric $BaTiO_3$ thin films.

DS 6.4 Tue 10:45 SCH A 315

Exploring transition-metal substitution in $FeSe_2$ thin films formed by seleniation at various temperatures — •Luqman Mustafa[1], Andreas Kreyssig[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Alfred Ludwig[2], and Anna E. Böhmer[1] — [1]Institute for Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, Germany

Transition-metal dichalcogenides with orthorhombic marcasite structure have been extensively studied for their applications in light energy conversion and photoelectrochemical devices. Lately this structure type has also gained interest for its magnetic properties as a candidate for the newly-predicted altermagnetic order.

Using combinatorial deposition and ex-situ selenization at 250°C, 350°C and 430°C, we have studied the substitution of iron with different TMs in (Fe,X)Se_2 thin films, (X= Co, Ni, Cr). This technique allowed to efficiently and quickly explore the possible ranges of substitution of TMs in this compound. We find that the marcasite structure of (Fe,Co)Se_2 forms with higher Co content when the selenization temperature is lower.

Our results represent an example for the agility of combinatorial deposition of thin films in exploring the phase diagrams of transition-metal dichalcogenides. It may be adapted for other systems, such as $FeSb_2$, and is therefore a unique tool to study a broad material family and its possible substitution ranges.

DS 7: 2D Materials and their Heterostructures IV

Time: Tuesday 11:15–12:30 Location: SCH A 316

DS 7.1 Tue 11:15 SCH A 316

THz-Light Canalization by means of Phonon Polaritons in 2D van der Waals Materials — •Maximilian Obst[1,2], Tobias Nörenberg[1,2], Gonzalo Álvarez-Pèrez[3], Thales V.A.G. de Oliveira[4], Alexey Nikitin[5], Pablo Alonso-González[3], J. Michael Klopf[4], Susanne C. Kehr[1,2], and Lukas M. Eng[1,2] — [1]TU Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence - EXC 2147 (ct.qmat), Germany — [3]University of Oviedo, Spain — [4]HZDR, Dresden, Germany — [5]DIPC, Donostia-San Sebastian, Spain

Hyperbolic phonon polaritons (PhP) in anisotropic, 2D van der Waals materials present a promising platform to shrink THz optics into nm-sized volumes, as they enable ultra-high field confinement. Recently, controlled PhP dispersion tuneability was demonstrated at MIR wavelengths by vertically stacking two α-MoO_3-flakes under a well-defined twist-angle θ, introducing a topological transition, where PhPs propagate along one distinct direction (so-called 'canalized propagation')[1].

In this talk, we explore the THz dispersion tunability in twisted bilayer MoO_3 at frequencies ranging from $\nu = 8.28$ to 9.38 THz, for which the existence of hyperbolic PhP has been demonstrated recently [2], and where longer (THz) wavelengths make strong confinement even more desirable. We demonstrate the transition from hyperbolic to elliptic propagation of these PhPs by varying both θ and ν and report the very first observation of canalized PhPs in the THz spectral range, i.e., for $\nu = 8.67$ THz and $\theta = 50°$.

[1] G. Hu et al., *Nature* **582**, 209 (2020).
[2] T.V.A.G. de Oliveira et al., *Adv. Mater.* **33**, 2005777 (2021).

DS 7.2 Tue 11:30 SCH A 316

Magnetically induced band splitting of the exfoliated antiferromagnet $MnPS_3$ revealed by temperature dependent μ-ARPES — •J. Strasdas[1], B. Pestka[1], M. Rybak[2], A. K. Budniak[3], N. Leuth[1], H. Boban[4], I. Cojocariu[4], D. Baranowski[4], V. Feyer[4], J. Avila[5], P. Dudin[5], Y. Amouyal[6], L. Plucinski[4], E. Lifshitz[3], M. Birowska[7], and M. Morgenstern[1] — [1]II. Institute of Physics B and JARA-FIT, RWTH-Aachen University, Germany — [2]Department of Semiconductor Materials Engineering Wrocław University of Science and Technology, Poland — [3]Schulich Faculty of Chemistry, Solid State Institute, Russell Berrie Nanotechnology insistute and Helen Diller Quantum Center, Technion, Israel Institute of Technology, Israel — [4]Forschungszentrum Jülich, Peter Grünberg Institute (PGI-6), Germany — [5]Synchrotron-SOLEIL, Université Paris-Saclay, France — [6]Department of Materials Science and Engineering, Technion, Israel Institute of Technology — [7]Institute of Theoretical Physics, University of Warsaw, Poland

We provide micron-scale angle-resolved photoelectron spectroscopy (μ-ARPES) of the exfoliated intralayer antiferromagnet (AFM) $MnPS_3$ above and below the Néel temperature in comparison with density functional theory (DFT) calculations. We demonstrate a splitting of parts of the Mn $3d_{z^2}$-bands induced by the AFM ordering in line with DFT results. Related changes of adjacent S 3p-bands indicate a competing FM superexchange contribution. This novel access to the electronic band structure is found to be transferable to other AFM MPX_3 materials (M: transition metal, P: phosphorus, X: chalcogenide).

DS 7.3 Tue 11:45 SCH A 316

Twistronics of high temperature superconductors — •Nicola Poccia — Leibniz Institute for Solid State and Materials Research Dresden (IFW-Dresden(

Ideally, one would like to have quantum technologies that could work at higher temperature and at the same time show all the advantages of a twisted architecture as for example its revolutionary degree of electronic tunability. However, highly tunable superconductors that operate above liquid nitrogen are either not yet showed up using multilayered graphene twisted heterostructures or the materials are very difficult to assemble in twisted heterostructures given their extreme sensitivity to the environmental conditions. Here we show a possible avenue towards the resolution of this problem, demonstrating how to engineer a new generation of the van der Waals heterostructures comprising atomically high temperature superconducting thin Bi2Sr2Can-1CunO2n+4 (where n = 1,2,3) crystals. The intended van der Waals constituent Bi2Sr2Can-1CunO2n+4 planes are twisted with respect to each other and make the Josephson junctions. We measure different quantum transport properties of the Josephson junctions in a wide range of twisted angles, indicating the high temperature superconducting topological nature of these systems. Finally, technological prospects on the realization of hybrid complex superconducting circuits will be given.

DS 7.4 Tue 12:00 SCH A 316

New magneto-polaron resonances in a monolayer of a transition metal dichalcogenide — Carlos Trallero-Giner[1,2], Darío G. Santiago-Pérez[3], and •Vladimir M. Fomin[1,4] — [1]Institute for Integrative Nanosciences (IIN), Leibniz IFW Dresden, D-01069 Dresden — [2]Havana University, Havana 10400, Cuba — [3]Universidad Autónoma del Estado de Morelos, CP 62209, Cuernavaca, Morelos, México — [4]Moldova State University, MD-2009 Chişinău, Republic of Moldova

For transition metal dichalcogenide (TMD) semiconductors, the behavior of the magneto-polaron resonances (MPRs) is revealed as a function of the phonon symmetry inherent in the system. It is shown that the renormalized Landau energy levels are modified by the interplay of the long-range Pekar-Fröhlich (PF) and short-range deformation potential (DP) interactions. This interplay leads to a new series of MPRs involving the optical phonons at the center of the Brillouin zone. The coupling of the two Landau levels with the LO and A_1 optical phonon modes provokes resonant splittings of double avoided-crossing levels giving rise to three excitation branches. To explore the interplay between the MPR, the electron-phonon interactions (PF and DP) and the couplings between adjacent Landau levels, a full Green's function treatment for the evaluation of the energy and its life-time broadening is developed. A generalization of the two-level approach is performed for the description of the new MPR branches. The obtained results are a guideline for the magneto-optical experiments in TMDs, where three MPR peaks should be observable.

DS 7.5 Tue 12:15 SCH A 316

Light driven magnetic transitions in transition metal dichalcogenide heterobilayers — •Michael Vogl[1], Swati Chaudhary[2,3,4], and Gregory Fiete[3,4] — [1]Department of Physics, King Fahd University of Petroleum and Minerals, 31261 Dhahran, Saudi Arabia — [2]Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA — [3]Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA — [4]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

We study strongly correlated phases of twisted transition metal dichalcogenide heterobilayers (tTMDs) subject to a period drive. Specifically, we employ Floquet theory to investigate how for this family of materials different forms of light can induce various magnetic phase transitions.

DS 8: Thin Film Properties III

Time: Tuesday 11:30–12:45 Location: SCH A 315

DS 8.1 Tue 11:30 SCH A 315

Growth of Sc(x)Ga(1-x)N on 6H-SiC by plasma assisted molecular beam epitaxy — •Fabian Ullmann[1,2], Aaron Giess[1,2], and Stefan Krischok[1,2] — [1]Institut für Physik, TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Institut für Mikro- und Nanotechnologien, TU Ilmenau, Gustav-Kirchhoff-Straße 7, 98693 Ilmenau

ScGaN can occure in different crystal orientations. Most important are the wurtzit and the rocksalt formation. In dependency of the Scandium concentration a phase tranistion between these orientations can be found.

Plasma assisted molecular beam epitaxy (PAMBE) in combination with reflective high electron energy diffraction (RHEED) was performed to create layers with different Scandium concentrations within ScGaN. To determine the concentration of the grown layers X-ray photoelectron spectroscopy (XPS) was used in the same vacuum chamber. Additionally, the surfaces were investigated by atomic force microscopy (AFM, in-situ) and scanning electron microscope (SEM) to gain information about the morphology of the surfaces and to confirm the gained crystal orientations investigations with X-ray diffraction (XRD) were made.

DS 8.2 Tue 11:45 SCH A 315

α-$FeGe_2$ films on GaAs(001) substrates grown by MBE and solid-phase epitaxy — •Moritz Hansemann, Michael Hanke, Achim Trampert, and Jens Herfort — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Layered magnets show promising results towards advancements in the field of spintronics. Such materials exhibiting a ferro- and/or antiferromagnetic (FM/AFM) phases close to room temperature are especially on demand for future technologies.

Recently we discovered a novel metastable α-$FeGe_2$ phase sandwiched between two ferromagnetic Fe_3Si Heusler alloy metals. Comprehensive transmission electron microscopy (TEM) and X-ray diffraction (XRD) measurements revealed the layered structure and P4mm spacegroup, that is absent in bulk $FeGe_2$. By a combination of molecular beam and solid phase epitaxy we demonstrate the isolated growth of α-$FeGe_2$ on a GaAs(001) substrate. This is achieved by first growing Fe_3Si and covering it with amorphous Germanium in the thickness ratio of 1:3. Finally, a subsequent annealing forms the layered $FeGe_2$. Through a optimization of this process we are able to grow layers of extremely high quality with layer thicknesses down to 4 nm. The films are structurally characterized by atomic force microscopy, XRD, X-ray reflectivity and TEM measurements, which also demonstrate the importance of a smooth GaAs initial surface. First transport measurements showed metallic behavior and a ferromagnetic behavior at low temperatures.

DS 8.3 Tue 12:00 SCH A 315

Heteroepitaxial Growth of Ultrawide Bandgap Cubic Spinel Zn_2GeO_4 Thin Films by Pulsed Laser Deposition — •Jingjing Yu, Sijun Luo, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig

It is significant to explore new ultrawide bandgap oxides thin films with a bandgap larger than 4 eV for potential applications in power electronics and deep-UV photodetectors. Cubic spinel Zn_2GeO_4 is a high-temperature and high-pressure phase which was originally synthesized at 1600 °C and 3 GPa. To date the experimental results on physical properties and thin film growth of cubic spinel Zn_2GeO_4 are not available. In this study, we report the heteroepitaxial growth of cubic spinel Zn_2GeO_4 thin films on cubic spinel $MgAl_2O_4$ single crystal substrates by using pulsed laser deposition at about 800 °C. Combining the analysis results from XRD 2theta-omega scans and rocking curves with the AFM surface morphologies, it is concluded that the oxygen partial pressure of around 0.05~0.10 mbar is optimal for growing high-quality Zn_2GeO_4 epitaxial thin films. Phi-scan results confirm the single-domain epitaxy of (100)-, (110)- and (111)-oriented Zn_2GeO_4 epitaxial thin films grown on (100), (110) and (111) $MgAl_2O_4$ substrates, respectively. The dielectric function of the cubic spinel Zn_2GeO_4 epitaxial thin films was measured by spectroscopic ellipsometry, indicating a bandgap energy greater than 4.5 eV. This work advances the fundamental research on ultrawide bandgap cubic spinel Zn_2GeO_4 epitaxial thin films.

DS 8.4 Tue 12:15 SCH A 315

Rutile $CuTiO_2$ alloy thin films: lowered growth temperature and retained optical properties. — •Hao Lu[1,2], Martin Becker[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), Justus-Liebig-University, Giessen, Germany

Titanium dioxide(TiO_2) with a rutile structure and suitable bandgap may be advantageously employed as buffer layer and anti-reflection layer in VO_2-based smart windows coated on float glass by sputter deposition. The phase transition of the thermodynamically metastable phases, anatase and brookite, into the stable rutile phase occurs in pristine TiO_2 at temperatures about 600°C, which is higher than the melting point of float glass. Hence, we need to significantly reduce the growth temperature of rutile TiO_2 in order to deposit it as the film on float glass substrates.

Cu doping has been reported as a means for achieving this goal. We study series of TiO_2:Cu thin-film samples deposited on float glass to assess the growth window for rutile TiO_2:Cu deposited at temperature below 600°C. The samples are compared with reference TiO_2 thin-films deposited under the same conditions in terms of crystal structure and optical properties.

DS 8.5 Tue 12:30 SCH A 315

The challenge to grow β-(AlxGa1-x)2O3 on (100) off-oriented β-Ga2O3 by MOVPE — •Jana Rehm, Ta-Shun Chou, Arub Akhtar, Raimund Grüneberg, Saud Bin-Anooz, and Andreas Popp — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Deutschland

Although immense progress in homoepitaxial thin film growth of β-Ga2O3 on different substrate orientations has been achieved, β-Ga2O3 based high-efficiency devices are still limited by the materials intrinsic low thermal conductivity and electron mobility. Increasing the bandgap by alloying β-Ga2O3 with Al2O3 opens up the possibility to overcome the materials restraints and realize high-performance lateral β-(AlxGa1-x)2O3/Ga2O3 heterostructure devices. It has been shown that the crystal orientation plays an important role in the Al incorporation limit and band offsets where the (100) orientation is predicted to be the most promising orientation exhibiting the highest critical thickness and incorporated Al content. The role of off-oriented (100) β-Ga2O3 substrates is suggested to achieve the full advantage of β-(AlxGa1-x)2O3/Ga2O3 heterostructure with the benefit of potentially suppressing the formation of twin defects. For the first time, we report a comprehensive study on the growth of β-(AlxGa1-x)2O3 on off-oriented (100) β-Ga2O3 substrates using MOVPE. The influence of different growth parameters on the morphology and Al incorporation are systematically investigated by HR-XRD and AFM.

DS 9: Layer Properties I

Time: Wednesday 9:30–10:30 Location: SCH A 316

Invited Talk DS 9.1 Wed 9:30 SCH A 316

Flüssigphasen-Elektrochemie im Ultrahochvakuum unter XPS-Kontrolle — •Frank Endres — Institut für Elektrochemie, TU Clausthal

Ionische Flüssigkeiten zeichnen sich durch zwei interessante Eigenschaften aus. Zum einen haben sie sehr weite sog. elektrochemische Fenster, die Untersuchungen ermöglichen, die insbesondere in wässrigen Elektrolyten nicht möglich sind. Zum anderen haben sie sehr geringe Dampfdrücke, die die Untersuchung ionischer Flüssigkeiten unter den Bedingungen eines Ultrahochvakuums ermöglichen. In diesem Beitrag werden nun beide Ansätze kombiniert, indem elektrochemische Prozesse in ionischen Flüssigkeiten im Ultrahochvakuum mittels Photoelektronenspektroskopie untersucht werden. Ein Einblick in die Prozesse bei der elektrochemischen Reduktion von Tantalverbindungen, in die Prozesse bei der elektrochemischen Oxidation von Gold sowie in Disproportionierungsreaktionen bei der Reduktion von Galliumverbindungen wird gegeben.

Literatur:

F. Krebs, O. Höfft, F. Endres, Applied Surface Science 155130 (2022)

Z. Liu, O. Höfft, A. Gödde, F. Endres, Journal of Physical Chemistry C 125 (2021) 26793*26800

Z. Liu, O. Höfft, F. Endres, Journal of Physical Chemistry C 125 (2021) 24589-24595

DS 9.2 Wed 10:00 SCH A 316

Oxide thickness-dependent resistive switching characteristics of Cu/HfO_2/Pt ECM devices — •Taewook Kim[1], Tobias Vogel[1], Eszter Piros[1], Despina Nasiou[2], Nico Kaiser[1], Philipp Schreyer[1], Robert Winkler[2], Alexander Zintler[2], Alexey Arzumanov[1], Stefan Petzold[1], Leopoldo Molina-Luna[2], and Lambert Alff[1] — [1]Advanced Thin Film Technology Division, Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [2]Advanced Electron Microscopy Division, Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

This study investigates the resistive switching mechanism and electrical conduction mechanism of the Cu/HfO_2/Pt MIM (Metal-Insulator-Metal) structure. In this study, we investigated the resistance switching characteristics of Cu/HfO_2/Pt samples. Specifically, we focus on changes in resistive switching characteristics as a function of oxide layer thickness. We noticed an interesting phenomenon of resistance switching property, that the reset switching occurs more sharply and abruptly in the sample with thick HfO_2 film. However, gradual reset is more dominant in the sample with thin HfO_2 film. Therefore, we devised the model (Thermally Assisted Electrochemical Mechanism) to explain the physical phenomenon. For better understanding, the conduction mechanism of Cu/HfO_2/Pt samples was also investigated. Cu/HfO_2/Pt has SCLC (Space Charge Limited Conduction) mechanism as the conduction mechanism. However, the mechanism is divided into several steps depending on the thickness of the oxide layer.

DS 9.3 Wed 10:15 SCH A 316

Substoichiometric conducting HfO_x phases as novel type of electrodes with a built-in oxygen vacancy reservoir for RRAM applications — •Philipp Schreyer[1], Nico Kaiser[1], Eszter Piros[1], Tobias Vogel[1], Taewook Kim[1], Despoina Nasiou[2], Leopoldo Molina-Luna[2], and Lambert Alff[1] — [1]Advanced Thin Film Technology Division, TU Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [2]Advanced Electron Microscopy Division, TU Darmstadt, Darmstadt, Germany

Hafnium oxide is an outstanding candidate as the active material in RRAM due to its performance and proven CMOS compatibility. In previous studies, we have shown that electrically conducting hafnium oxide phases can be stabilized by significant oxygen deficiency [1,2]. While so far only the physical properties of these structures have been investigated, we reproduced the phases in RRAM configuration to investigate the device properties. Resistive switching was found to be absent in all deficient in-vacuo processed samples. They show ohmic conduction, confirming the conducting nature of the substoichiometric phases. However, when exposed to air, a thin oxidized layer forms at the surface which stabilizes reliable resistive switching. Note that the oxidation process is self-limited leading to reproducible oxide thicknesses of a few nm. We suggest that the substoichiometric phases may act as second electrode with an oxygen vacancy reservoir that stabilizes oxygen vacancy filaments in ultrathin layers of near-stoichiometric HfO_2. [1] N. Kaiser et al., ACS Appl. Mater. Interfaces 14, 1290 (2022). [2] N. Kaiser, accepted. ACS Appl. Electron. Mater. (2023).

DS 10: Layer Properties II

Time: Wednesday 11:00–12:15 Location: SCH A 316

DS 10.1 Wed 11:00 SCH A 316

Electronic structure of epitaxial (Cr1-xMnx)2GaC thin films by X-ray absorption and optical spectroscopy — •Ivan Tarasov[1], Andrei Rogalev[2], Fabrice Wilhelm[2], Michael Farle[1], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]The European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France

Heteroepitaxial thin films of (Cr1-xMnx)2GaC MAX phase for x = of 0.13 - 1 were deposited on MgO(111), Al2O3(0001) and KAl3Si3O10(001) substrates by pulsed laser deposition at T = 500-600 °C. X-ray absorption near edge spectroscopy (XANES) spectra were collected at the Mn K-edge, Cr K-edge and Ga K-edge. Evidence of chemical disorder associated with (Mn, Cr) is observed. The similarity of the Cr K-edge spectra to Mn, and the presence of a strong X-ray linear dichroism signal for the Mn K-edge, indicates that Mn is substitutional for Cr in the MAX phase hexagonal lattice. With increasing of Mn content additional features attributed to a cubic antiperovskite structure are observed. Simulations of the XANES spectra confirm the origin of X-ray linear dichroism observed in the sample, which is due to the inherent nanolaminated structure of the MAX phase.

Funding by the Deutsche Forschungsgemeinschaft (DFG) within CRC/TRR 270, project B02 (Project-ID 405553726) is gratefully acknowledged. We thank Martina Schmid (University of Duisburg-Essen) for assistance and providing access to the ellipsometer.

DS 10.2 Wed 11:15 SCH A 316

Perovskite-organic multiple quantum wells towards lasing — •Tobias Antrack[1], Martin Kroll[1], Markas Sudzius[1], Changsoon Cho[1], Paulius Imbrasas[1], Miguel Albaladejo-Siguan[1], Johannes Benduhn[1], Lena Merten[2], Alexander Hinderhofer[2], Frank Schreiber[2], Sebastian Reineke[1], Yana Vaynzof[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Dresden, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

Metal halide perovskites are of high interest due to their excellent electro-optical properties. Their high damage threshold makes them of special interest for high-fluence applications like lasing devices, and the possibility of production by vacuum deposition is promising for future large-scale industrial production. This technique allows precise thickness control and, therefore, the production of multiple quantum wells (MQWs). Such structures result in high charge carrier concentration and enhanced electron-hole recombination, making them promising for high-performance and fine-tunable materials. This work presents a comprehensive study of the optical properties of vacuum-deposited $CsPbBr_3$ perovskite MQWs with organic (TPBi) barrier layers. Blue shifts in absorption and emission spectra with decreasing well width demonstrate quantum confinement and are confirmed by simulations. Additionally, the photoluminescence quantum yield increases by up to 32 times from bulk material to the thinnest well layers. Amplified spontaneous emission (ASE) measurements show very low thresholds down to 7.3 μJ cm^{-2} for a perovskite thickness of 8.7 nm, which is significantly lower than previously observed for $CsPbBr_3$ thin films.

DS 10.3 Wed 11:30 SCH A 316

Defect-engineered magnetic field dependent optoelectronics of vanadium doped tungsten diselenide monolayers — •Christin Mädler[1,2], Katharina Nisi[1,2], Jonas Kiemle[1,2], Lukas Powalla[3], Alessio Scavuzzo[3], Tuan Dung Nguyen[4,5], Dinh Loc Duong[4,5], Marko Burghard[3], Alexander W. Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center of Quantum Science and Technology (MCQST), Schellingstrasse 4, 80799 Munich, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [4]Center for Integrated Nanostructure Physics (CINAP), Institut for Basic Science (IBS), Suwon 16419, Republic of Korea — [5]Department of Energy Science, Sungkyunkwan University, Suwon 16419, Republic of Korea

In this work, we investigate semiconducting WSe_2 monolayers, substitutionally doped with vanadium atoms, using low temperature luminescence and optoelectronic spectroscopy. V-dopants lead to a p-type doping character and an impurity-related emission $\sim$ 160 meV below neutral exciton, both of which scale with the nominal percentage of vanadium dopants. Measurements using field-effect devices of 0.3% V-doped WSe_2 demonstrate bipolar carrier tunability. The doped monolayers display a clear magnetic hysteresis in photocurrent measurments for the studied range of carrier densities, whereas the valley polarization of the excitons reveals a non-linear g-factor without a magnetic hysteresis within the experimental uncertainty.

DS 10.4 Wed 11:45 SCH A 316

On the influence of the cation composition in reactively co-sputtered $Ag_xCu_{1-x}I$ thin films: Characterization of electrical, optical and structural properties — •Sofie Vogt, Christiane Dethloff, Jorrit Bredow, Tillmann Stralka, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Germany

CuI and its alloys are promising transparent p-type materials for complementary transparent devices. Polycrystalline thin films exhibit hole mobilities of about 19 cm^{2}V^{-1}s^{-1}, which is comparable to the electron mobility of commercially used indium-gallium-zinc-oxide thin films[1,2]. It has been shown that alloying CuI with Ag leads to a transition from p-type material to n-type material for $x \approx 0.5$[3]. This paves the way for $Ag_xCu_{1-x}I/Ag_yCu_{1-y}I$ based homojunction diodes. We present reactively co-sputtered $Ag_xCu_{1-x}I$ thin films in a range of $0.01 \leq x \leq 0.86$. The thin films were deposited on glass substrates and crystallized in the γ-phase up to $x \leq 0.67$ and exhibit an additional AgI phase for higher Ag contents. An increase of the thin film resistivity from $2 \times 10^{-4}\,\Omega$m to 30 Ωm was achieved by increasing the silver content from $x = 0.01$ to $x = 0.67$. All thin films are transparent in the visible light range and the expected decrease of the exciton binding energy up to $x \approx 0.5$ is observed, above which it remains constant.

[1] C. Yang *et al.*, ACS Appl. Electr. Mater., 2, 3627-3632, 2020.
[2] S. Yang *et al.*, IEEE Electron Device Lett., 32 (12), 1692-1694, 2011.
[3] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.

DS 10.5 Wed 12:00 SCH A 316

Novel Energy-Filtered Field Stop Technology For Highly Blocking IGBTs — •Robert Koch[1], Marcel Gerold[1], Shavkat Akhmadaliev[2], Michael Rüb[1], and Elke Wendler[3] — [1]Ernst-Abbe-Hochschule, Fachbereich SciTec, Jena, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Friedrich-Schiller-Universität, Physikalisch-Astronomische Fakultät, Jena, Germany

Insulated Gate Bipolar Transistors (IGBTs) require on the one hand adjustable switching behavior and on the other hand high blocking capability. The technology presented in this work aims at implementing continuous deep carrier profiles as field stop structures. We insert a micro-patterned silicon membrane (energy filter) into the primary ion beam. This broadens its energy spectrum in a well controlled way, allowing production of extended continuous profiles. The micro patterns are restricted to rectangular shapes, due to the KOH etching manufacturing process. This means, instead of using multiple implantation steps for field-stop formation, our approach results in tailored smooth profiles by using energy-filtered Hydrogen implantations in the range of 1500 to 2500 keV. The defect profiles generated by H-implantation, are transformed into hydrogen-related donors by annealing at 300 to 400 °C. The annealing efficiency is related to the implanted dose (10^{13} to 5×10^{15} cm^{-2}), annealing temperature, hold time and the process gas composition (H_2 content 2 %). The defect profiles caused by proton bombardment using an energy filter and subsequent annealing are analyzed by Spreading Resistance Profiling (SRP).

DS 11: Thin Film Application

Time: Wednesday 11:00–12:15 Location: SCH A 315

DS 11.1 Wed 11:00 SCH A 315

Resonante Mikrowellenabsorberschichten für Fusionsreaktoren — •Andreas Hentrich — Universität Stuttgart

Um einen Fusionsreaktor zu betreiben wird ein Heizsystem benötigt, im Falle des ITERs ist das eine Mikrowellenheizung bei 170GHz. Dies impliziert aber direkt, dass entsprechende Absorber vorhanden sein müssen, die den extremen Bedingungen innerhalb eines Fusionsreaktors standhalten. Ebendiese wurden für den ITER in Form einer gemischten Metall-Oxid-Schicht realisiert. Da geläufige Mikrowellenabsorber platzintensiv sind, wurde ein resonanter Absorptionsmechanismus genutzt, was Absorptivitäten von über 90% bei Schichtdicken von rund 100μm ermöglicht.

Der Absorptionsmechanismus wurde sowohl im Modell als auch durch Messungen verifiziert und quantifiziert. Es wurden die Reflektivitäten von vier verschiedenen Materialsystemen winkel-, schichtdicken- und polarisationabhängig bestimmt. Deren Materialeigenschaften wurden mit Hilfe der Modelle bestimmt und damit die Schichten hinsichtlich ihrer Absorptionseigenschaften optimiert.

DS 11.2 Wed 11:15 SCH A 315

The effect of photon recycling and back-grading on CIGS cell performance — •Seçil Güler[1,2], Uwe Rau[1,3], and Thomas Kirchartz[1,2] — [1]IEK-5 Photovoltaik, Forschungszentrum Jülich — [2]NST and CENIDE, Universität Duisburg-Essen — [3]Faculty of Electrical Engineering and Information Technology, RWTH Aachen University

Photon recycling, i.e. the reabsorption of photons created by radiative recombination within the solar cell, is the missing link between Shockley-Queisser model and classical diode theory. In order to determine the thermodynamic limits of solar cells, it is therefore necessary to consider the photon recycling process. This study aims at calculating the theoretical efficiency limits of Cu(In,Ga)Se2 (CIGS) solar cells using 1-dimensional drift-diffusion solvers by including the effect of photon recycling and bandgap grading. Simulations of current-voltage curves were performed by changing limiting factors such as back grading, back surface recombination velocity, electron and hole mobilities, and Shockley-Read-Hall (SRH) lifetime as well as the back reflection at the interface of the Mo/CIGS structure. We investigate under which circumstances photon recycling has a significant effect on device performance and study the optimum bandgap grading for different material properties.

DS 11.3 Wed 11:30 SCH A 315

Strategies to obtain chiral perovskites via surface modification — •Markus Heindl[1,2], Tim Kodalle[3], Natalie Fehn[2], Lennart Reb[2], Shangpu Liu[1,2], Constantin Harder[2,4], Maged Abdelsamie[3], Lissa Eyre[2,5], Ian Sharp[2], Stephan Roth[4,6], Peter Müller-Buschbaum[2], Alexander Urban[7], Aras Karouzian[2], Carolin Sutter-Fella[3], and Felix Deschler[1] — [1]Heidelberg University, Heidelberg, Germany — [2]Technical University of Munich, Garching, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [5]University of Camebridge, Camebridge, Great Britain — [6]KTH Royal Institute of Technology, Stockholm, Schwede, — [7]Ludwig-Maximilians-Universität, Munich, Germany

The generation, manipulation and detection of light is a key requirement for a wide range of technologies. Thus, this field is in the constant focus of further technological advancement. Recent discoveries on the design of chiral metal-organic perovskites now promise cheap, sustainable materials for energy efficient generation and detection of polarized light. However, so far, the available pool of chiral perovskite materials is limited to a few one- and two-dimensional crystal structures.

Here, we present novel strategies to produce perovskite thin films with chiral surface modification directly. The resulting compound displays strong circular dichroism effects in the blue spectral region, which can be adjusted in their intensity by varying synthetic parameters. Furthermore, we perform an extensive structural investigation into the origin of these phenomena utilizing XRD and GIWAX experiments.

DS 11.4 Wed 11:45 SCH A 315

All-oxide thin-film varactors with Mn- and Ni-doped (Ba,Sr)TiO_3 for microwave applications — •Yating Ruan[1], Stipo Matic[2], Alexey Arzumanov[1], Philipp Komissinskiy[1], Rolf Jakoby[2], and Lambert Alff[1] — [1]Advanced Thin Film Technology, Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany — [2]Microwave Engineering and Technology, Technische Universität Darmstadt, Darmstadt, Germany

With a trend toward miniaturization of modern electronics, tunable microelectronic devices operating over a wide range of frequencies are required for mobile communications, high-speed data connections with the upcoming 5G and Internet of Things (IoT) technologies.

Here we present all-oxide thin-film tuneable capacitors (varactors) with single-crystalline films of a tunable dielectric perovskite $Ba_xSr_{1-x}TiO_3$(BST) doped with Mn and Ni, grown epitaxially by pulsed laser deposition on a highly conducting thin-film oxide $SrMoO_3$ bottom electrodes with a room-temperature resistivity of 30 $\mu\Omega$cm. A partial substitution of the tetravalent Ti at B-sites of the BST perovskite structure with Mn and Ni in a trivalent or divalent state decreases a concentration of oxygen vacancies in the BST, leading to a reduction of the leakage current density of the varactor by 5 orders of magnitude down to 1 A/m^2. The low leakage current allows the thickness of the BST layers to go below 50 nm, enabling varactors tunable with low voltages.

DS 11.5 Wed 12:00 SCH A 315

Finite Volume Modeling of Two-Dimensional Memristive Devices for Neuromorphic Computing — •Benjamin Spetzler[1], Dilara Abdel[2], and Patricio Farrell[2] — [1]Technische Universität Ilmenau, Ilmenau, Germany — [2]Weierstrass Institute, Berlin, Germany

In recent years, memristive devices have shown considerable potential for realizing synaptic functionalities in neuromorphic computing systems. Here, we present numerical models to analyze the hysteretic behavior of memristive devices. A finite volume model self-consistently solves the semiconductor equations for the electrostatic potential and the quasi-Fermi levels of electrons and holes. Further, we include the dynamics of mobile dopants and briefly discuss the boundary conditions implemented for the calculation of the switching dynamics and the current-voltage characteristics. Simulations are compared with measurements on two-dimensional flake devices based on MoS2. The results are used to validate the simulations and discuss the underlying switching mechanisms. Implications for the design of memristive devices are derived and discussed.

This work was partially funded by the Carl-Zeiss Foundation via the Project MemWerk and the German Research Foundation (DFG) through the Collaborative Research Centre CRC 1461 "Neurotronics - Bio-Inspired Information Pathway" as well as the Leibniz competition.

DS 12: Poster

Time: Wednesday 17:00–19:00 Location: P3

DS 12.1 Wed 17:00 P3

Growth and structural investigation of the SnBiTe stoichiometric series via MBE and TEM — •Xiao Hou[1], Abdur Rehman Jalil[2], Detlev Grützmacher[2], Claus Claus Michael Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6, Forschungszentrum Jülich, Germany — [2]PGI-9, Forschungszentrum Jülich, Germany

A topological phase transition (TPT) can be induced to engineer the band structure. This TPT is a fascinating, yet complex phenomenon in condensed matter research. Upon changing the stacking order of layers having different spin-orbit coupling (SOC) strengths, one can achieve a topological phase transition between trivial and nontrivial states [1,2]. Here, the $Sn_xBi_yTe_z$ (SBT) stoichiometric series is a classical example, in which a stacking-dependent topological phase transformation group is explored.

The epitaxial growth of three distinct compositions i.e. $SnBi_2Te_4$, $SnBi_4Te_7$, $Sn_2Bi_2Te_5$ is conducted on Si (111) substrates via molecular beam epitaxy (MBE). X-ray diffraction (XRD) is employed to characterize the crystal quality of the grown thin films. We have also used advanced transmission electron microscopy (TEM) to investigate the stacking order. High-angle annular dark-field imaging provided detailed information about the crystallinity and atomic arrangements of the layer stacks and also of various types of structural defects in the thin films. The link between the stacking order and the topological characteristics requires further investigation that is ongoing.

[1] B.-J. Yang and N. Nagaosa, Nature Comm. 5, 4898 (2014). [2] R. Peng et al. Phys. Rev. B 101,115427 (2020).

DS 12.2 Wed 17:00 P3

Thin film growth characterization of a mulitpurpose physical vapor deposition apparatus with the goal of investigating tailored perpendicular magnetic anisotropy systems — •Florian Ott, Christian Janzen, Arne Schröder, and Arno Ehresmann — Institute of Physics, University of Kassel, D-34132 Kassel

In recent years, systems of multilayered (ML) magnetic thin films consisting of ferromagnetic transition metals (TM) with noble metallic spacers displaying perpendicular magnetic anisotropy (PMA) have gained increased interest for applications in magnetic particle transport [1], controlled domain movement [1,2] and sensor technologies [3]. These TM-based PMA systems may rely on the precise modulation of layer growth additionally to the already very low thickness requirements [1]. As a result, a precise control of the growth conditions is necessary in order to produce these systems. This work focuses on the characterization of growth conditions and parameters inside a multipurpose physical vapor deposition (PVD) apparatus with the ultimate goal of creating and investigating engineered TM-based PMA systems. [1] M Urbaniak, et al. Magnetization reversal of Co/Au multilayer stripes with keV-He+ ion bombardment induced coercivity. J. Phys. D: Appl. Phys. 48 (2015) 335003 (7pp) gradient, [2] A. Jarosz, et al. Magnetic domain propagation in Pt/Co/Pt micro wires with engineered coercivity gradients along and across the wire, Journal of Magnetism and Magnetic Materials, Volume 435 (2017) [3] M. Matczak, et al. Co/Au multilayers with graded magnetic anisotropy for magnetic field sensing. applied physics letters 100, 162402 (2012)

DS 12.3 Wed 17:00 P3

Strain and Lattice-Relaxation Effects of (Al,Ga)N/GaN Interfaces on 4D-STEM Signals — •Frederik Otto, Laura Niermann, Tore Niermann, and Michael Lehmann — Technical University of Berlin, Berlin, Germany

The immense increase in computation power over the past decades can be attributed to the decreasing size of semiconductor device structures. Preceding this trend, semiconductor research focuses on thin films and their interfaces with the surrounding substrate material.

At these interfaces of heterogeneous device structures, the atomic lattices are strained due to the mismatch of lattice constants of interfacing materials. Scanning-Transmission Electron-Microscopy (STEM) is capable of resolving strain at a nanometer scale, however, investigated specimens must be sufficiently thin to be electron transparent. For such thin specimens, the relaxation of the strained lattice at its surfaces cannot be neglected when measuring strain in an electron microscope.

Here, knowledge about the underlying strain and relaxation effects at the interface of (Al,Ga)N/GaN Quantum Wells (QWs) is obtained by comparing 4D-STEM measurements with simulations. By carefully choosing the experimental parameters, i.e., convergence angle and tilt, features of multiple scattering events are found in the measured diffraction discs perpendicular to the QW structure at every position of a 2D scanned area. These features are evaluated by comparison with corresponding simulations considering a strain field and relaxation effects as obtained from finite element calculations.

DS 12.4 Wed 17:00 P3

Comparative evaluation of EDS quantification methods for the analysis of $Sc_xAl_{1-x}N$ films — •Hauke Honig[1], Rebecca Petrich[2], Lorenz Steinacker[1], Younes Slimi[2], Daniel Glöss[3], Stephan Barth[3], Hagen Bartzsch[3], Raphael Kuhnen[4], Dietmar Frühauf[4], Stefan Krischok[2], and Katja Tonisch[2] — [1]Technische Universität Ilmenau, Fachgebiet Werkstoffe der Elektrotechnik, IMN MacroNano®, 98693 Ilmenau — [2]Technische Universität Ilmenau, Fachgebiet Technische Physik I, IMN MacroNano®, 98693 Ilmenau — [3]Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik FEP, 01277 Dresden, Germany — [4]Endress+Hauser SE+Co. KG, TTD Technologieentwicklung, 79689 Maulburg, Germany

The quantitative analysis of $Sc_xAl_{1-x}N$ films with energy dispersive x-ray spectroscopy (EDS) poses some challenges due to peak overlaps and the thin film character. Standard-free and standard-based methods are compared regarding their reliability for the quantification of the Sc-content in sputtered films with $0 \leq x \leq 0.35$ and evaluated using reference samples that have been quantified with GDOES and EDS by Fraunhofer FEP. Therefore, parameters such as acceleration voltage, selection of standard materials and quantification models are considered. Theoretical spectrums generated with Monte-Carlo simulations are used to improve the selection of excitation energy in the small range between substrate influence and limits of the quantification models. The crystalline hexagonal structure is confirmed with XRD.

DS 12.5 Wed 17:00 P3

From Doping to Dilution: Local Chemistry and Collective Interactions of La in HfO_2 — •Oliver Rehm[1], Thomas Szyjka[1,2], Lutz Baumgarten[2], Claudia Richter[3], Yury Matveyev[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[1] — [1]Uni Konstanz, Konstanz, Germany — [2]FZJ, Jülich, Germany — [3]NaMLab, Dresden, Germany — [4]DESY, Hamburg, Germany — [5]TU Dresden, Dresden, Germany

HfO_2-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or FeFET. The application of HfO_2-based thin films as active ferroelectrics (FE) in these devices face reliability issues like wake-up, imprint, and fatigue. The FE phase of HfO_2 is the metastable orthorhombic structure, for which La doping is considered a promising route for stabilization.

La:HfO_2 samples were grown by ALD with a range of La doping, from 3.5% to 33%, i.e., from the doping to dilution level. We link the local chemistry at the La lattice sites with local and collective electronic properties of the La:HfO2 matrix using HAXPES. The satellite structure of La 3d core level, the plasmonic excitation energies, and core-level rigid binding energy (BE) shifts are investigated. The emerging chemical phases and electronic properties are discussed as a function of La doping. From the evolution of the plasmon excitation energies and rigid BE shifts, it is concluded that electronic charge compensation by oxygen vacancies occurs for increasing La content.

[1] T. Szyjka, et al., Phys. Status Solidi RRL 2022, 16, 2100582

DS 12.6 Wed 17:00 P3

Molecular Dynamics - Two Temperature Model simulations of gold — •Othmane Benhayoun[1], Emiliano Principi[3], Bernd Bauerhenne[1], Dmitry S. Ivanov[2], and Martin E. Garcia[1] — [1]University of Kassel, Theoretical physics II, Kassel, Germany — [2]Moscow, Russia — [3]Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

We aim to explain the results obtained from a recent Ultrafast Electron Diffraction (UED) experiment that showed periodic oscillations in both height and width of the (311) Au diffraction peak. The same

effect is however not observed in polycrystalline gold. We have thus performed Molecular Dynamics - Two Temperature Model (MD-TTM) simulations to model more than 11 million atoms, enabling us to understand the underlying physical processes. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics.

DS 12.7 Wed 17:00 P3

In situ X-Ray Total Scattering Investigation of Thermal Annealing in FeCoSiB Metallic Glass Films — •Nicolas Hayen[1], Philipp Jordt[1], Lars Thormählen[2], Mathis Mewes[1], Ann-Christin Dippel[3], Olof Gutowski[3], Niklas Wolff[2], Lorenz Kienle[2], and Bridget Murphy[1,4] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Institute of Material Sciences, Kiel University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [4]Ruprecht Haensel Laboratory, Kiel University, Germany

Thin films of the iron-based metallic glass $(Fe_{0.9}Co_{0.1})_{78}Si_{12}B_{10}$ (FeCoSiB) are seen as a promising candidate for technical applications in high sensitivity magnetic field sensors and have been utilized extensively within the CRC 1261 "Biomagnetic Sensing". Thermal annealing of these films leads to a decrease in quality of the desired magnetic properties depending on the parameters of the annealing process.
In situ grazing incidence high-energy x-ray total scattering experiments were used to investigate the onset of structural changes occurring in the material. Films of thickness ranging from 0.05 to 1μm were investigated under varied annealing conditions with temperatures up to 700°C. From these measurements we were able to observe two separate crystallization phase transitions and the emergence of textured structures. Further analysis of the scattering from the amorphous phase may give further insight into the initial structural changes the material undergoes during annealing and their influence on magnetic properties.

DS 12.8 Wed 17:00 P3

Synthesis of structurally defined graphene nanoribbons: Peritetracene and it's corresponding 1,1'-bitetracene precursor — •Maren Klein[1,2], John B. Bauer[2], Marie Wagner[1,2], Holger F. Bettinger[2], Thomas Chassé[1], and Heiko Peisert[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany — [2]Institute of Organic Chemistry, University of Tübingen, Germany

Band gap engineering of precise nanographenes has attracted much attention in the field of organic electronics as they show great electronic properties. One class of these promising nanographenes are acenes and their related peri-acenes. Acenes are linearly condensed polycyclic hydrocarbons whereas peri-acenes exhibit a two-dimensionally enlarged π system. As peri-acenes possess a diradical open-shell character, the synthesis is quite challenging. Here we demonstrate that peritetracene can be formed on-surface by annealing the deposited precursor molecule 1,1'-bitetracene on a Cu (111) surface. The unique 1,1'-bitetracene undergoes a surface-assisted cyclodehydrogenation which was investigated by microscopic and spectroscopic techniques, as well as by DFT calculations. In the XAS spectra we could observe that the as-deposited molecule shows a vanishing intensity of π^* transitions at normal incidence (90°), which indicates a planarization of the molecule already before annealing and an almost flat lying adsorption geometry.

DS 12.9 Wed 17:00 P3

Study of cadmium-based thin films obtained by pulsed laser deposition — •Cristina Postolachi[1], Georgiana Bulai[1], Sandu Cibotaru[2], Alexandru Cocean[1], Bogdanel Silvestru Munteanu[3], Nicanor Cimpoesu[1,4], Silvia Garofilde[1], Georgiana Cocean[1], Iuliana Cocean[1], and Silviu Gurlui[1] — [1]Alexandru Ioan Cuza University of Iasi, Faculty of Physics, Atmosphere Optics, Spectroscopy and Laser Laboratory (LOASL), 11 Carol I Bld. 700506 Iasi, Romania — [2]Petru Poni Institute of Macromolecular Chemistry, Gr. Ghica Voda Alley, 41A, 700487 Iasi, Romania — [3]Alexandru Ioan Cuza University of Iasi, Faculty of Physics, 11 Carol I Bld. 700506 Iasi, Romania — [4]Gheorghe Asachi Technical University of Iasi, Faculty of Material Science and Engineering, 59A Mangeron Bld., Iasi, Romania

This study investigates the processes that occur when different chemical compounds of cadmium are mixed with selenium and are further used as targets for thin film growth by pulsed laser deposition. Here the interactions between these compounds in the laser induced plasma plume will be analyzed.

The aim of the investigation of the reactions that take place in the plasma plume at high vacuum is to obtain thin films of cadmium selenide. The thin films proprieties will be investigated with different techniques, such as Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDX), X-ray Diffraction (XRD), profilometry, UV-VIS spectroscopy and others.

DS 12.10 Wed 17:00 P3

Fabrication of copper halide thin films by combinatorial PLD — •Christopher Walter, Felix-Florian Delatowski, Michael Bar, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Copper halides are promising p-type materials for transparent device applications due to their large direct band gaps ($E_g = 3{-}3.4\,eV$) [1]. Here we present the deposition of copper halide thin films by combinatorial pulsed laser deposition (PLD) and discuss their structural, morphological and optical properties as a function of different growth parameters [2]. At ambient conditions, CuI crystallizes in the cubic zinc-blende structure. XRD shows <111>-orientation for CuI independent from the used substrate material. CuBr and CuCl grow polycrystalline with the same crystal structure as CuI. However, with the incorporation of low iodine concentration, the crystallinity improves significantly. We find that the thin films exhibit very smooth surfaces with a roughness of $R_{RMS} = 0.8{-}1.6\,nm$ for the binary CuI, CuBr and CuCl systems under optimal parameters. Furthermore, using combinatorial PLD and a segmented target with one segment each of CuBr and CuI, ternary $CuBr_xI_{1-x}$ alloys were grown. Based on the resulting locally varying composition, the influence on structural and optical properties can be directly observed.
[1] M. Grundmann *et al.* : phys. stat. sol. (a) 210, 9, 1671 (2013)
[2] H. von Wenckstern *et al.* : phys. stat. sol. (b) 257, 7, 1900626 (2019)

DS 12.11 Wed 17:00 P3

Electrical characterization of SnTe thin film topological crystalline insulator — •Negin Beryani Nezafat, Sepideh Izadi, and Gabi Schierning — Department of physics, Experimental physics, Bielefeld University, 33615, Bielefeld, Germany

Topological crystalline insulators (TCIs) with gapless metallic states and protected carrier transport offer unique electrical features. Band structure of these materials consists of conventional parabolic band diagram together with linear surface transport. In this work, SnTe thin film as a promising TCI is considered to be our model system. Therewith, SnTe thin films with different thicknesses are deposited on silicon substrate using RF magnetron sputtering. The resulting morphology characterization for rock-salt SnTe crystalline thin film fulfills stoichiometric ratio. Electrical characterization including temperature dependent resistivity, magnetoresistance and Hall analysis are performed using Van der Pauw configuration. These findings introduce SnTe thin film as a promising candidate for technical applications such as device fabrication.

DS 12.12 Wed 17:00 P3

Current probe AFM measurements on reactively co-sputtered $Ag_xCu_{1-x}I$ thin films — Tillmann Stralka, •Sofie Vogt, Christiane Dethloff, Jorrit Bredow, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Germany

CuI exhibits a high hole mobility of up to $44\,cm^2/Vs$ in bulk crystals and of about $19\,cm^2/Vs$ in polycrystalline thin films[1,2]. This, combined with high transparency in the visible light range, renders CuI an interesting material for transparent complementary devices. However, grain boundary (GB) conduction is dominating electrical properties and might inhibit device performance[3]. Annadi *et al.* showed that alloying with silver reduces the conductivity of $Ag_xCu_{1-x}I$ thin films and even results in switching from p-type to n-type[4].

We present topological and current probe (cp)-atomic force microscopy measurements on reactively sputtered $Ag_xCu_{1-x}I$ thin films with silver contents from x=0.1 to x=0.6. A strong decrease of the grain size with increasing silver content is observed. In addition, a decrease of the overall surface current is observed, which agrees well with electrical bulk characterizations. For $x \geq 0.39$ we observed that the current from tip to sample is mainly injected at grain boundaries while for large Ag content the injected current at GBs is negligible.
[1] D. Chen *et al.*, Crystal Growth Design, 10, 2057*2060, 2010.
[2] C. Yang *et al.*, ACS Appl. Electr. Mater., 2, 3627-3632, 2020.
[3] Kneiß *et al.*, Adv. Mater. Interfaces, 5, 1701411, 2018.

[4] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.

DS 12.13 Wed 17:00 P3

Analysis of the structural properties of $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_{2-\delta}$ (NCM) thin film model cathodes — Julius Konstantin Dinter and •Matthias Elm — Center for Materials Research, Justus-Liebig-University Giessen Germany, Heinrich-Buff-Ring 16, 35392 Giessen

Lithium ion batteries often suffer from capacity fading due to undesired side reactions occurring at the cathode surface. To get a deeper understanding of these side reactions, 2D model system are necessary. For this purpose, NCM thin film cathodes were prepared via spin coating followed by annealing at high temperatures. Using these thin film cathodes allow us to perform various surface sensitive measurements such as Raman microscopy, AFM, ESM, SEM and EDX. As no additives are used, we are able to study the surface reaction occurring at the cathode active material in more detail using in-situ measurements. The results reveal structural changes of the surface accompanied by an increase of the cell resistance, which confirms the formation of an SEI. Furthermore, the electrochemical performance of thin films coated with Al_2O_3 using atomic layer deposition (ALD) were investigated. The analysis of the surface properties confirm that coating of the NCM-thin film suppresses the undesired surface reactions resulting in an improved long-term cycling stability.

DS 12.14 Wed 17:00 P3

Nanoscopic Investigation of the Monolayer $MoSe_2$-WSe_2 Lateral Heterostructures under Illumination — •Alexander Turchanin[1], Tobias Nörenberg[1], Ziyang Gan[2], Antony George[2], Andrey Turchanin[2], Susanne C. Kehr[1,3], and Lukas M. Eng[1,3] — [1]TU Dresden — [2]Friedrich Schiller University Jena — [3]Wuerzburg-Dresden Cluster of Excellence - EXC 2147 (ct.qmat)

Transition metal dichalcogenides (TMDCs) such as $MoSe_2$ and WSe_2, are inorganic semiconductor monolayers with great potential for integration into nanoscale devices. Monolayers of different TMDCs can be engineered into lateral or vertical heterostructures forming, e.g., 1D or 2D p-n junctions that strongly respond to light [1]. Here, lateral heterostructures of monolayer $MoSe_2$ and WSe_2 grown by chemical vapor deposition are studied at the nanometer length scale by Kelvin Probe Force Microscopy (KPFM) under visible to near-infrared light illumination, i.e. photon energies between 1.45 and 1.95 eV. This approach enables for the simultaneous recording of both the sample surface morphology and the local photoinduced surface potential. By employing the side-band KPFM demodulation [2], quantification of the local band-bending of this in-plane heterostructure is possible with superior sensitivity. Different alterations of the local surface potential are observed when choosing the light exposure above and below the individual TMDCs bandgap energies.

[1] P.A. Markeev et al., *J. Phys. Chem. C* **125**, 13551 (2021).
[2] T. Wagner et al., *Beilstein J. Nanotechnol.* **6**, 2193 (2015).

DS 12.15 Wed 17:00 P3

Electronic structure of MXenes determine from angle-resolved photoelectron spectroscopy — •Wei Yao[1], Dongqi Li[1,2], Jonas A. Krieger[1], Mihir Date[1], Emily C. McFarlane[1], Minghao Yu[1,2], Xinliang Feng[1,2], and Niels B.M. Schröter[1] — [1]Max-Planck Institute of Microstructure Physics, Halle (Saale), 06120, Germany — [2]Center for Advancing Electronics Dresden (cfaed) and Faculty of Chemistry and Food Chemistry, TU Dresden, Dresden, 01062, Germany

Transition metal carbides, also known as MXenes, have been one of the most fascinating two-dimensional material systems beyond graphene. Chemical substitution of the transition metal elements and terminal function groups have resulted in versatile and tunable electronic, optical and mechanical properties, with applications in energy storage, multifunctional sensors, transparent and flexible electrodes, electromagnetic interference shielding, or hydrogen evolution reaction catalysis [1]. However, to reveal the origins of the MXenes' exceptional properties, a deeper understanding of their electronic structure is required. Here we report the first micro-focused angle-resolved photoemission spectroscopy (ARPES) measurements of single MXene flakes, which will reveal the influence of the chemical environment on the the single-particle electronic band structure, as well as many-body effects reflected in its spectral function.

[1]. A. VahidMohammadi, J. Rosen, and Y. Gogotsi. The world of two-dimensional carbides and nitrides (MXenes). Science 372, eabf1581 (2021)

DS 12.16 Wed 17:00 P3

Mode-selective Raman Signal Enhancement in MoS_2/WS_2 Heterostructures — •Annika Bergmann[1], Mustafa Hemaid[1], Rico Schwartz[1], Ziyang Gan[2], Antony George[2], Andrey Turchanin[2], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany

In the family of van der Waals materials, transition metal dichalcogenides (TMDCs) have attracted much attention in recent years. Stacking various TMDC materials forms heterostructures in which new phenomena, such as interlayer charge transfer and interlayer excitons [1] occur. However, for the observation of interlayer effects good contact between the constituent monolayers is crucial.
Here, we investigate bilayer heterostructures that were formed by combining Chemical Vapor Deposition (CVD) grown MoS_2 and exfoliated WS_2 monolayers. Photoluminescence quenching is used as an indicator to evaluate the interlayer coupling. In addition, the out-of-plane (A_{1g}) phonon mode provides information on the interfacial contact [2]. We observe a selective enhancement of the WS_2 A_{1g} Raman mode in well-coupled MoS_2/WS_2 heterostructures compared to WS_2 monolayers or heterostructures with only poor contact. A systematic study of this phenomenon is presented to elucidate its microscopic origin.

[1] Fang et al., Proc. Natl. Acad. Sci. USA 111 (2014)
[2] Zhou et al., ASC Nano 8 (2014)

DS 12.17 Wed 17:00 P3

Exfoliation of 2D materials for nanooptics — •Jakob Wetzel[1], Maximilian Obst[1,2], Susanne C. Kehr[1,2], and Lukas M. Eng[1,2] — [1]TU Dresden, Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence - EXC 2147 (ct.qmat), Dresden, Germany

The desire for smaller and more energy efficient optical components leads to the necessity of light confinement below the diffraction limit. This can be achieved e.g by phonon polaritons (PhPs) which are quasiparticles formed by the coupling of infrared photons with the optical phonons of a crystal. Particularly the related light confinement is enhanced when the PhPs are generated in anisotropic, 2D van der Waals materials such as MoO_3 and GeS [1, 2]. Therefore, flat and μm - sized nanosheets of such materials are required, which can be realized by mechanical exfoliation.

Here, we present an optimized exfoliation technique for MoO_3 and GeS resulting in the reproducible generation of 20 to 100 μm - sized flakes with a thickness of about 100 nm. We present a quick and easy to implement adaptation of the scotch-tape exfoliation technique as well as exemplary results based on optical microscopy images and atomic force microscopy.

[1] T.V.A.G de Oliveira et al., *Adv. Mater.* **33**, 2005777 (2021).
[2] T. Nörenberg et al., *ACS Nano*, published online (2022), DOI: 10.1021/acsnano.2c05376.

DS 12.18 Wed 17:00 P3

hybrid resonant circuits with van der Waals materials — •haolin jin[1], giuseppe serpico[2], christian n. saggau[2], sanaz shokri[2], mickey martini[2], yejin lee[2], poya yang[1], sebastian seifert[1], uri vool[1], and nicola poccia[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibnitz Institute for Solid State and Materials Science Dresden (IFW Dresden), Dresden, Germany

Van der Waals superconductors, especially heterostructures, are believed to exhibit novel superconducting phases. However, the standard measurement techniques designed for bulk superconductors are challenging to apply in 2D materials which cannot be grown in sufficient size and quality. Herein, we introduce an efficient method to explore the properties of 2D materials, by combining them into hybrid resonant circuits. The resonator can have a strong inductive interaction with a small-size superconducting sample, affecting its frequency response. However, creating superconducting contacts between the resonator and the 2D material is challenging, especially for air-sensitive materials where evaporation must be done in a protected glovebox. Here, we present a technique to make robust superconducting contacts to a 2D sample by using a flexible nanomembrane. The Niobium resonator circuit is fabricated on top of the nanomembrane, and via contacts connect it to the 2D materials. Through the circuit response, we can explore the properties of novel unconventional superconductors. Moreover, this hybrid circuit is a new type of quantum device for future quantum technology applications.

DS 12.19 Wed 17:00 P3

Phase transformations in few-layer transition metal phosphorus trichalcogenides studied by low-voltage TEM — •Alexander Storm[1], Janis Köster[1], Mahdi Asl-Gohrbani[2], Silvan Kretschmer[2], Tatiana Gorelik[1], Michael K. Kinyanjui[1], Arkady Krasheninnikov[2], and Ute Kaiser[1] — [1]Central Facility Materials Science Electron Microscopy, Ulm University, 89081 Ulm, Germany, — [2]Institute of Ion Beam Physics and Materials Research, Helmholt-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany,

In this work we study phase transformations in freestanding few-layer transition metal phosphorus trichalcogenides (TMPTs) induced by electron irradiation as well as thermal annealing in vacuum, using various analytical transmission electron microscopy techniques (TEM). In addition, our results are supported by ab-initio calculations.

We show that due to knock-on damage, first sulphur atoms are ejected in sulphur-based TMPTs at common TEM acceleration voltages (60kV - 300kV), which in turn leads to the formation of defects and strong modifications of the TMPT's properties [1]. For instance, we show that in few-layer MnPS3 and MnPSe3, stable, ultrathin α- and γ-MnS/MnSe phases are formed showing the reliability of this transformation in Mn based TMPTs. Eventually, we elucidate the emerging phases and transition temperatures for few-layer MnPS3, MnPSe3, FePS3, FePSe3, and NiPS3 induced by thermal annealing.

[1] Köster, Storm et al., J. Phys. Chem. C, 126, 36, 15446 (2022).

DS 12.20 Wed 17:00 P3

Encapsulating high-temperature superconducting twisted van der waals heterostructures blocks detrimental effects of disorder — •Yejin Lee[1,2], Mickey Martini[1,2], Tommaso Confalone[1], Sanaz Shokri[1,2], Christian Saggau[1], Daniel Wolf[1], Genda Gu[3], Kenji Watanabe[4], Takashi Taniguchi[4], Domenico Montemurro[5], Valerii Vinokur[6], Kornelius Nielsch[1,2], and Nicola Poccia[1] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY, USA — [4]NIMS, Tsukuba, Japan — [5]University of Naples Federico II, Naples, Italy — [6]Terra Quantum AG, Gallen, Switzerland

Van der Waals (vdW) heterostructures based on cuprate superconductors attract substantial interest of novel topological phases as well as technological applications. One of the hindrances for the progress is the detrimental effect of disorder on the properties of the vdW devices-based Josephson junctions. This work reports a novel method of fabricating twisted vdW heterostructures made of Bi2Sr2CuCa2O8+x, combining the employed cryogenic stacking using a solvent-free stencil mask technique and additionally covering the interface with insulating hexa boron nitride layers. We find that encapsulating the interface in the stacked systems overcomes detrimental effects of disorder providing highly coherent Josephson junction. This finding enables crucial improvement of its critical current and the Tc of the junctions up to their magnitudes in bulk intrinsic junctions.

DS 12.21 Wed 17:00 P3

In-situ formation of Mo_6Te_6 nanowire in single-layer 2H-$MoTe_2$ by annealing and electron irradiation — •Janis Köster[1], Silvan Kretschmer[2], Michael K. Kinyanjui[1], Alexander Storm[1], Fabian Rasper[1], Arkady V. Krasheninnikov[2], and Ute Kaiser[1] — [1]Electron Microscopy of Materials Science, Ulm University, Albert Einstein Allee 11, 89081 Ulm, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Up to now, the fundamental understanding of transformations in 2D materials at the atomic scale are not fully characterized. Here, we demonstrate a route to locally transform freestanding single-layer (1H-) $MoTe_2$ [1] into 1D-Mo_6Te_6 nanowires [2] under electron beam irradiation and by heating. (HR)TEM at the Cc/Cs-corrected SALVE [3] microscope at 80 kV is used to analyse structural changes in the material. Combining the experimental data with the results of first-principles calculations, we explain energetics and stabilities of $MoTe_2$ monolayers and Mo_6Te_6 nanowires due to an interplay of electron-beam-induced energy input, atom ejection, and oxygen absorption. A detailed understanding of high-temperature solid-to-solid phase transformation in the 2D limit provides insights into the material's applicability for future device fabrication.

[1] J. Köster, et al. The Journal of Physical Chemistry C 125.24 (2021): 13601-13609.
[2] H. Kim, et al. Small 16.47 (2020): 2002849
[3] M. Linck, et al. Physical review letters 117.7 (2016): 076101

DS 12.22 Wed 17:00 P3

structural and magnetic properties of two dimensional (2D) Fe_xGeTe_2 and Fe $_xGaTe_2$ grown by molecular beam epitaxy (MBE) — •Atekelte Kassa, Hua Lv, Neha Aggrawal, Michael Hanke, Abbes Tahraoui, Manfred Ramsteiner, and Marcelo Lopes — Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Berlin, Germany

2D materials with intrinsic functionality showed importance in fundamental condensed-matter science and for the development of advanced technologies, where 2D ferromagnetic materials have raised interest for developing low dimensional magnetic/spintronic devices. Yet maintaining 2D ferromagnetism at /above room temperature remains a challenge. This work presents our recent results on 2D ferromagnets of Fe_xGeTe_2 and Fe $_xGaTe_2$ ($3 \leq x \leq 5$) prepared using MBE. Films were grown at 300 °C using elemental fluxes of Fe, Ge (Ga), and Te on epitaxial graphene on SiC (0001). Epitaxial films with good structural quality were confirmed by reflection high-energy electron diffraction and X-ray Diffraction. Atomic force microscopy confirmed continuous and smooth surface growth. Raman spectroscopy results showed that the graphene layers remain structurally unaltered after MBE growth. Anomalous Hall effect investigations through Magneto-transport studies identified a perpendicular magneto anisotropy as well as a Curie temperature (T_c) above 300 K for both films with Fe composition close to x=5. For Fe $_xGaTe_2$, T_c values around 380 K were obtained. These results make the studied ferromagnets promising for the development of novel spintronic devices based on 2D materials and heterostructures.

DS 12.23 Wed 17:00 P3

Towards engineering of tailored 2D single photon emitters (SPE) by encapsulating single dye molecules into few layer hexagonal boron nitride (hBN) — •Nils le Coutre, Tim Völzer, Paul Weinbrenner, Lisa Böhme, Franziska Fennel, Tobias Korn, Stefan Lochbrunner, and Friedemann Reinhard — University of Rostock, Rostock, Germany

We hypothesize that encapsulating dye molecules into multilayer hBN flakes overcomes photobleaching, for example by improved thermal conduction and airtight sealing. This would tackle one of the biggest barriers to the application of fluorescent dyes in various methods like optical nearfield microscopy or quantum sensing. I will present work to deposit dyes on exfoliated multilayer hBN flakes by different methods of physical vapor deposition (PVD) and liquid deposition, as well as initial studies on photostability by confocal microscopy. The large variety of available dye molecules will provide a rich toolbox for engineering of 2D SPEs, with greater flexibility than the limited set of intrinsic defects in 2D materials and bulk crystals.

DS 12.24 Wed 17:00 P3

Epitaxy and transfer of freestanding oxide perovskites — •Jeremy Maltitz, Duc Nguyen, Alev Yuvanc, Jens Martin, and Jutta Schwarzkopf — Leibniz Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Deutschland

Fabrication of artificial 3D heterostructures is of increasing interest for a broad range of application, such as flexible sensor, memristors, or electronic skins. Layer transfer of thin films has established a new paradigm of material assembly and design in context of 2D-van-der-Waals crystals. Recently, freestanding oxide perovksites have been achieved by introducing a perovskite-like sacrificial layer (Sr3Al2O6) between substrate and functional film. In combination with layer transfer, the functional film can be placed on arbitrary substrates (e.g. silicon wafers). Additionaly, two functional layers (same or different) can be stacked with the opportunity to create moiré patterns by rotating the layers with respect to each other. Therefore, the influence of PLD growth parameter and thickness of SrTiO3/Sr3Al2O6 heterostructures are studied to improve the quality of freestanding SrTiO3 thin films. Furthermore, the solid-solution family of (Ba,Ca,Sr)3Al2O6 enables the possibility to tune the lattice parameter. This property was used to adjust the lattice parameter of the sacrificial layer to closely match the lattice parameter of SrTiO3. With improved growth parameter and lattice matched sacrificial layer, the crackformation of the freestanding film was reduced, paving the path towards the stacking of freestanding thin films.

DS 12.25 Wed 17:00 P3

Characterization of structural and magnetic properties of

$SrRuO_3$ thin films — •Vitor de Oliveira Lima[1], Mai Hussein Hamed[1], Connie Bednarski-Meinke[1], Michael Faley[2], Emmanuel Kentzinger[1], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institute (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH, Germany. — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ERC), Forschungszentrum Jülich GmbH, Germany.

Proximity effects in Ferromagnet/Superconductor Heterostructures (F/S-H) have demonstrated high potential for development of new devices for spintronic and quantum computing application. $SrRuO_3$ (SRO) has attracted much attention among transition metal oxides for being the only 4d oxide to show itinerant ferromagnetism and metallic conductivity. In this work, we are characterizing the crystal structure as well the magnetic properties of SRO thin films for further application in F/S-H with $YBa_2Cu_3O_{7-x}$ superconducting films. The samples were prepared on STO (001) single crystals by High-Oxygen Pressure Sputtering. SRO thin films are epitaxial and have smooth surface. Magnetometry indicate that samples have out-of-plane magnetic anisotropy and paramagnetic-ferromagnetic transition at approximately 150 K, which corresponds to the SRO with Ru^{4+} Curie temperature, and two transitions at lower temperatures, that may be related to another Ru oxidation state. The samples stoichiometry will be further investigated by Rutherford Backscattering Spectroscopy.

DS 12.26 Wed 17:00 P3

Charge-to-spin conversion in the quasi-two-dimensional electron gas emerging at the doped interface between $LiNbO_3$ and $LaAlO_3$ — •Igor Maznichenko[1,2], Sergey Ostanin[1], Ingrid Mertig[1], and Paweł Buczek[2] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]Department of Engineering and Computer Sciences, Hamburg University of Applied Sciences, Berliner Tor 7, D-20099 Hamburg, Germany

We anticipate that the functional use of a solid electrolyte lithium niobate in $LaAlO_3/LiNbO_3$ heterostructure allows one to tune the quasi-two-dimensional electron gas (q2DEG) which emerges there. This phenomenon can be achieved by charging and discharging $LiNbO_3$. Here, on the basis of *ab initio* calculations of the hydrogen-doped $LaAlO_3/LiNbO_3$ interface, we demonstrate how the q2DEG and its spin polarization appear. The out-of-plane electric polarization of $LaAlO_3/LiNbO_3$ forces the H dopants to accommodate at the Al-terminated interface. This results in the formation of the q2DEG, whose spatial extent is about 1.5 nm along the stacking direction.

DS 12.27 Wed 17:00 P3

Preparation of oxide ferroelectric membranes by epitaxial sacrificial layers — •Jonas Wawra[1,2], Robin Adlung[1,2], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]Institute for Metallic Materials, Leibniz IFW Dresden, Germany — [2]Institute of Applied Physics, TU Dresden, Germany

Oxide ferroelectric thin films are used in a variety of applications due to their strong remnant polarization and excellent dielectric, piezoelectric and optoelectric properties. However, well performing and robust materials require a high crystalline quality and orientation, which is commonly achieved by growing the desired ceramic on comparably thick and rigid substrates at high temperatures. This procedure prohibits in most cases the incorporation in advanced organic heterostructures and limits their utilization in flexible devices. One idea to overcome the discrepancy between processing and implementation is the use of a sacrificial layer during growth, which allows to release the functional material as a thin membrane afterwards and enables a transfer to flexible substrates. Here, we present our approach by growing different fully epitaxial hetero-structures of $La_{0.7}Sr_{0.3}MnO_3$ (which can be wet-etched in a hydrochloric acid solution), conducting $SrRuO_3$ and ferroelectric $Ba_{1-x}Sr_xTiO_3$ on oxide single crystal substrates by pulsed laser deposition. Different sample architectures were used to obtain a diversity of membranes that allow us to study their microstructure and functional properties with methods like X-ray diffraction, scanning probe microscopy, dielectric and ferroelectric measurement techniques to compare them to similar films still clamped on a substrate.

DS 12.28 Wed 17:00 P3

Resistive switching and oscillations in $NdNiO_3$ and $SmNiO_3$ planar thin film devices — •Farnaz Tahouni-Bonab[1], Theodor Luibrand[1], Claribel Domínguez[2], Jennifer Fowlie[2], Stefano Gariglio[2], Rodolfo Rocco[3], Soumen Bag[3], Lorenzo Fratino[3], Marcelo Rozenberg[3], Jean-Marc Triscone[2], Reinhold Kleiner[1], Dieter Koelle[1], Javier del Valle[2], and Stefan Guénon[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) an LISA$^+$, Universität Tübingen, 72076 Tübingen, Germany — [2]Department of Quantum Matter Physics, Université de Genève, 1211 Geneva, Switzerland — [3]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France

Recently, there has been growing interest in strongly correlated materials that undergo a temperature-driven insulator-to-metal transition in the emerging research field of neuromorphic computing. Of particular interest are resistive switching phenomena for emulating integrate-and-fire behavior or self-sustained oscillations for spike train generation. In this study, we used a combination of wide field microscopy and electrical transport measurements to investigate thin film devies of the charge transfer insulators $NdNiO_3$ and $SmNiO_3$. Current-voltage characteristics and photomicrographs reveal resistive switching via an intermediate state with a blurry metallic filament. The intermediate state is accompanied by oscillations in the 10 kHz frequency range that have a characteristic saw-tooth shape indicative of a relaxation oscillator. The intermediate state can be suppressed by changing the slew rate of the current source.

DS 12.29 Wed 17:00 P3

Determining the brazeability of copper surfaces via spectroscopic ellipsometry — •Friedrich Bürger, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

In Brazing, surface conditions play a fundamental role in determining the joint strength. Not all changes of the surface, like thick oxide layers or oil films, may be immediately apparent and therefore will only be noticed when the brazing process failed. Since most methods of determining brazeability work by performing a brazing process and evaluating the results they can only be performed on samples. This does not represent variation of surfaces within a batch of material. To fill this gap a nondestructive method to determine brazeability is needed. Spectroscopic ellipsometry (SE) is an optical measurement method commonly used to characterize the optical properties of surfaces and thin films. To evaluate if SE can be used to distinguish surface states of copper surfaces that negatively impact the joint strength, different surfaces were prepared. The selected surface states were a reference condition, ground surfaces, oxidized surfaces and different oil films on the reference surface. Those surfaces were characterized by confocal laser scanning microscopy (CLSM) and X-Ray photoelectron spectroscopy (XPS) to determine their morphology and chemical composition. SE-measurements were performed subsequently. Except for the ground states all surfaces showed distinct features in their SE-spectra, suggesting identification via SE is possible.

DS 12.30 Wed 17:00 P3

Microscopic theory of X-ray absorption spectroscopy — •Joris Sturm, Dominik Christiansen, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS) are two widely used methods to investigate the structure of solid states. [1,2,3].
In this contribution, we present a self-consistent Maxwell-Bloch approach based on Heisenberg equations of motion for a unified description of XANES and EXAFS for 2D solid-state materials and apply it to the exemplary material graphene. For XANES we reproduce the experimentally observed absorption peaks and polarization-dependent selection rules of the included orbitals. Furthermore, the rigorous treatment of the Bloch wave interference allows us to calculate the Fourier transformed EXAFS spectrum [2] predicting so far uninterpreted features which have not been assigned within point-scattering theory [1].

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[2] Buades, Bárbara, et al., Optica 5 (2018): 502
[3] Chowdhury, M. T., R. Saito, and M. S. Dresselhaus, PRB 85 (2012): 115410.

DS 12.31 Wed 17:00 P3

Ultrafast vibrational dynamics of CH-stretch modes of surface adsorbates — •Tim Lämmerzahl, Nelli Kremer, and Eckart Hasselbrink — University Duisburg-Essen

The understanding of energy transfer between different modes in one molecule, which is called internal vibrational energy redistribution

(IVR), is crucial for further development in the field of rate theory and for applications in molecular electronics. As a model we study adsorbate monolayers of a single species using time-resolved two-color pump probe sum frequency spectroscopy.
Previously, we revealed that the coupling between valence vibrations is faster than a few ps and equilibrates with bending and torsion modes on a tens of ps time scale in fatty acid monolayers [1]. Now we moved on to conducting surfaces (e.g. gold) and used different terminated alkanethiols. Since gold surfaces exhibit a strong non-resonant (NR) signal, which is usually the dominant source of noise, we used the technique by Dlott et al.[2] to suppress the NR signal. Results from a study of alkylthiols with different headgroups on gold will be presented.

[1] Lackner, M., Hille, M., Hasselbrink, E. (2019), Phys. Chem. Lett., 11, 108-112.
[2] Lagutchev, A., Hambir, S. A., Dlott, D. D. (2007). J. Phys. Chem. C., 111, 13645-13647.

DS 12.32 Wed 17:00 P3

Dynamics of the response of thiol monolayers to rapid heating — •Matthias Linke and Eckart Hasselbrink — Universität Duisburg-Essen, 45141 Essen, Germany

Energy transport between metal substrates and molecules as well as intramolecular energy transport between vibrations is still not well understood, even though systems such as thiols on gold were studied extensively. Self-assembled molecular films are an ideal model system such as their characterization attracted much interest over the last decades, especially in the field of nanotechnology. It is well established that thiols adsorb easily and reproducibly on gold substrates by self-assembly. Sum-frequency generation vibrational spectroscopy (SFGvS) can be used for characterization of such systems, since it is inherently sensitive to surface species, interfaces at which centrosymmetry is broken. We adsorbed different thiols on Au-surfaces and heated the substrate by focussing an additional 25 ps 532 nm laser beam on the backside of the sample. Absorption of the photons leads to temperature jumps in the metal which can be assessed by tracking the reflectivity changes of the sample. Tracking the spectral changes via SFGvS at different delays between the pump and probe pulses can be done to assess the temperature effects induced in the substrate and the molecules and time constants can be extracted. The effect of the probing of different head groups (NO_2, CN, CH_3) and variation of the spacer group are studied in this work.

DS 12.33 Wed 17:00 P3

In-situ spectroscopic ellipsometry measurement and analysis of native SiO2 behavior under different atmosphere and temperature — •Younes Slimi[1,2], Jannis Waldmann[1], Rüdiger Schmid-Gund[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Strafte 32, 98693 Ilmenau, Germany — [2]Ferhat Abbas University, Institut of optics and precision mechanics, Optics and Applied Photonics laboratory 19000 Setif, Algeria

the most common wafer used in the semiconductor industry nowadays is silicon (Si), the latter oxidizes when left to its own devices. these silicon oxide layers' behavior was investigated using In-situ Spectroscopic ellipsometry to obtain optical constants and thin film thicknesses under different atmospheres (nitrogen, dry air) and temperatures. We found changes in the refractive index and thickness of the SiO2 layer under different conditions due to oxidation and material ablation. These results are meant to be used as possible references for future Electrochemical cells for in-situ Spectroscopic ellipsometry measurement for water splitting devices.

DS 12.34 Wed 17:00 P3

Sprayed hybrid nanocellulose fibril-silver nanowire transparent electrodes — •Marie Betker[1,2], Constantin Harder[1,3], Elisabeth Erbes[1,4], Julian Heger[3], Alexandros E. Alexakis[2,5], Benedikt Sochor[1], Qing Chen[1], Matthias Schwartzkopf[1], Andrei Chumakov[1], Peter Müller-Buschbaum[3,6], Konrad Schneider[7], Simone Techert[1], L. Daniel Söderberg[2,5], and Stephan V. Roth[1] — [1]DESY, 22607 Hamburg — [2]Fibre and Polymer Technology, KTH, 10044 Stockholm, Sweden — [3]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [4]Institute for X-ray Physics, Goettingen University, 37077 Goettingen — [5]WWSC, KTH, 10044 Stockholm, Sweden — [6]MLZ, TUM, 85748 Garching — [7]Leibniz-Institut für Polymerforschung Dresden e.V., Abteilung Werkstofftechnik, 01069 Dresden

The fabrication of sustainable, thin, and flexible electrical devices on an industrial scale will be an important challenge in the future. Nanocomposites, consisting of conductive nanoparticles like silver nanowires (AgNWs) and a sustainable matrix material like cellulose nanofibrils (CNFs), can meet these requirements. Here, we report on the nanoscale structure and the corresponding optoelectronic properties of a sprayed CNFs-AgNWs nanocomposite electrode. Adding CNF to the aqueous AgNW-based spray ink improves the dispersion and distribution of the AgNWs. This, and the cold-welding of the AgNW junctions enhance the conductivity of the electrode greatly. Finally, we demonstrate the electrode's high transmittance, resilience under multiple cycles of bending deformations, and its long-term stability.

DS 12.35 Wed 17:00 P3

Detecting nitrogen-vacancy-hydrogen centers on the nanoscale using nitrogen-vacancy centers as local sensors in CVD-diamond — •Christoph Findler, Gerhard Wolff, Karolina Schüle, Rémi Blinder, Priyadharshini Balasubramanian, Johannes Lang, Christian Osterkamp, and Fedor Jelezko — Institute for Quantum Optics, Ulm University, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

The negatively-charged nitrogen-vacancy center (NV) in diamond has attracted a lot of attention in the field of quantum technologies as it shows coherence times up to milliseconds at room temperature and enables optical polarization and coherent control of the electron spin. Apart from NV centers, the spin bath in diamond grown by chemical vapor deposition (CVD) consists mainly of substitutional nitrogen (P1) and negatively charged nitrogen-vacancy-hydrogen (NVH) defects which are usually analyzed by electron paramagnetic resonance (EPR) spectroscopy. In nm-thick epitaxial layers, however, the total number of paramagnetic spins becomes eventually too low for state-of-the-art EPR spectrometers. This problem can be solved by switching to a confocal microscope and studying the NV centers optically. Here, we show that 15NV ensembles can be employed as local sensors to estimate the density of non-fluorescent 15NVH and P1 centers in 15N-doped (100)-diamond layers and even get insight into the spatial distribution and correlation of P1 and 15NVH on the micrometer scale using a wide-field microscope.

DS 12.36 Wed 17:00 P3

Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution — •Mahdad Mohammadi, Ruiwen Xie, Niloofar Hadaeghi, Aldin Radetinac, Alexey Arzumanov, Philipp Komissinskiy, Hongbin Zhang, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt

$SrMoO_3$, $SrNbO_3$, and $SrVO_3$ are remarkable highly conducting d^1 (V, Nb) or d^2 (Mo) perovskite metals with an intrinsically high transparency in the visible. A key scientific question is how the optical properties of these materials can be manipulated to make them suitable for application as transparent conductors and emergent plasmonics. In this work, it is demonstrated for the first time how $3d/4d$ cationic substitution in perovskites shifts the optical transition energy and plasma frequency. At the example of the solid solution $SrV_{1-x}Mo_xO_3$ we show that the absorption and reflection edges can be shifted to the edges of the visible, resulting in a material that has the potential to outperform ITO due to its extremely low sheet resistance. For $x = 0.5$, a resistivity of 32 *Ωcm (12 Ω/sq.) is paired with a transmittance above 84 % in the whole visible spectrum. Quantitative comparison between experiments and electronic structure calculations show that the shift of the plasma frequency is governed by the interplay of d-band filling and electronic correlations.

[1] M. Mohammadi *et al.*,"Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution", Adv. Mater. (2022), Accepted Author Manuscript 2206605

DS 12.37 Wed 17:00 P3

Influence of dielectric Layers on the optomechanical Properties of Polymer Membranes in a Fiber Cavity — •Andreas Reuss[1], Stefan Linden[1], Hannes Pfeifer[2], Lukas Tenbrake[2], and Alexander Fassbender[1] — [1]Physikalisches Institut, Universität Bonn, Germany — [2]Institut für Angewandte physik, Universität Bonn, Germany

Fiber cavities are an attractive platform for optomechanical experiments as they can combine direct fiber-coupled optical access, small cavity lengths, high optical finesse, and an open resonator volume. Direct laser writing allows for a fast and flexible way to add polymer

drums as mechanical resonators directly on the end facets of a fiber cavity. These membrane-in-the-middle systems show a rather large optomechanical coupling strength despite of the low reflectivity due to the maximized intensity differences on the two membrane interfaces. A disadvantage of direct laser written structures are the comparatively large mechanical losses of the used resist, which limit the mechanical quality factor of the membranes to several hundred at cryogenic temperatures. Therefore, we are interested how the deposition of different dielectric layers influences the optomechanical response of the polymer membranes. By using materials with high young's modulus, like MgF_2, we aim to reduce overall mechanical losses and therefore increase the optomechanical response.

DS 12.38 Wed 17:00 P3

IST 312 - an unconventional phase change material? — •Maria Häser, Peter Kerres, Sophia Wahl, Carl-Friedrich Schön, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany

Chalcogenide-based Phase Change Materials (PCM) are a prominent candidate for energy-efficient memory devices. This material class shows a significant difference in its optical properties between the amorphous and crystalline phases: The former phase shows more insulating characteristics. In contrast, the almost metallic properties characterise the crystalline state. However, enabling fast switching between insulators and a real metal would broaden the field of application of PCMs.

In this study, the unusual phase change material In_3SbTe_2 (IST) has been investigated, which shows a metallic-like behaviour in its crystalline phase. The dielectric functions of both phases were determined using optical measurements (FTIR, Ellipsometry). Additionally, DFT calculations and XRD measurements were performed to better understand the unusual property change.

DS 12.39 Wed 17:00 P3

Characterization of the interaction of acrylic polymers with gold and silica surfaces — •Sascha Jan Zimmermann, Philipp Moritz, and Wolfgang Maus-Friedrichs — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Adhesives play a key role in the 21st century. In particular, hybrid material composites can be joined in this way while saving weight. To advance this technology, a fundamental understanding of adhesive interactions, particularly to metal (oxide) substrates, is required.

In order to investigate these interactions, nanometer thin planar polymer films were deposited on the model substrates of silicon oxide and gold. This was done for the polymers poly(methyl methacrylate) and poly(glycidyl methacrylate) applying a spin coating process. X-ray photoelectron spectroscopy (XPS), Metastable Impact Electron Spectroscopy (MIES) and Ultraviolet photoelectron spectroscopy (UPS) were used to analyze the chemical interactions at the interface.

In the case of PMMA, the XPS measurements show the presence of a caboxylate ion, which indicates probable ionic interactions. A varying chemical shift and the changes in the MIES spectra indicate additional hydrogen bonds. In the case of PGMA, no interactions were detected by the applied measurement methods.

DS 12.40 Wed 17:00 P3

Photoinduced charge injection into single-layer WSe2 via deposited dye molecules — •Tim Völzer[1,2], Alina Schubert[1,2], Julian Schröer[1], Rico Schwartz[1], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institute of Physics, University of Rostock, Albert-Einstein-Str. 23, 18059 Rostock, Germany — [2]Department "Life, Light and Matter", University of Rostock, Albert-Einstein-Str. 25, 18059 Rostock, Germany

The deposition of molecules allows the functionalization of 2D semiconductors as well as the fabrication of hybrid structures exhibiting charge separation after optical excitation that can be exploited in optoelectronic devices. Here, we investigate the charge transfer from optically excited molecules of the dye Perylene Orange (PO) into a monolayer of tungsten diselenide (1L-WSe_2) by means of low-temperature micro-photoluminescence spectroscopy: In comparison to the blank 1L-WSe_2, the proportion of charged trion versus neutral exciton emission is expected to change as the PO molecules are deposited and excited. In contrast, when reducing the pump photon energy below the PO absorption band, the emission spectrum would remain identical. Thus, we aim to control the light-induced charge injection into the WSe_2 by tuning the pump wavelength.

DS 12.41 Wed 17:00 P3

Theoretical insights into the monolayer adsorption and characterization of HB238 Merocyanine on Ag(100) surface — •Ritu Tomar, Thomas Bredow, Anna Kny, and Moritz Sokolowski — Clausius Institute of Physical and Theoretical Chemistry, University of Bonn, Germany

Merocyanines (MCs) are intriguing compounds that can be used as efficient absorbers for organic solar cells. We studied the adsorption of HB238 merocyanine on the surface of Ag (100) using STM and SPA-LEED experiments, which suggested that HB238 self-organizes as chiral tetramers upon adsorption. The molecular structure was significantly different from the typical configuration in the bulk phases of HB238. It is critical to control the structure and morphology of merocyanine films to enhance light absorption and optimize their optoelectronic properties. Therefore, we performed quantum chemical calculations to corroborate our experimental findings. Initially, we screened the HB238 conformers and used the most stable structure to determine the optimal adsorption orientation of HB238 on the Ag surface using the semi-empirical method GFN1-XTB in DFTB+. HB238 preferentially adheres face-on to the Ag surface. Next, we optimized the tetramer models at the DFT level to analyze the assembly of chiral tetramers while maintaining supercell lattice constant values, as in the experiment. We then relaxed the HB238 molecules on the Ag 3-layer slab model and fixed the bottom two layers using the GGA method in VASP. However, rapid and effective system convergence was achieved only using the ASE/LBFGS optimization algorithm.

DS 12.42 Wed 17:00 P3

Modelling liquid flow through nanopores on the nanoscale — •Rustam Durdyyev[1], Christian R. Wick[1], and Ana-Sunčana Smith[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, PULS Group, Institute for theoretical physics, Interdisciplinary Center for Nanostructured Films (IZNF), Cauerstrasse 3, 91058 Erlangen, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia

Liquid chromatography is one of the most important separation techniques and has proceeded mainly along empirical knowledge from the expansive collection of experimental data by using chromatographic methods, spectroscopic methods and technical innovations in column packing, particle technology and equipment design. However, a classic liquid chromatography column, is a cylinder densely packed with mesoporous silica particles whose surface has been mostly chemically modified. In this work, we investigated the physisorption of water to functionalized silica surfaces and hydrophilicity properties of surface by molecular dynamics simulations. We built on previously gathered knowledge on chromatography to establish a unified picture of stationary phase and solute mobility in liquid chromatography. In analogy to previous studies, we utilized a crystalline SBA-15 structure as starting point for our modeling approach. Furthermore, we investigate the effect of functionalization using different loadings with silanol group (Si-OH) and trimethylsilyl groups (O-SI-(CH3)3). With this strategy, we hope to understand the effect of functionalization of silica on the physisorption of water molecules at the nanometer scale.

DS 12.43 Wed 17:00 P3

Optimizing two-dimensional materials for biomolecule detection using machine learning techniques — •Calin-Andrei Pantis-Simut[1,2,3], Amanda Teodora Preda[1,2,3], Nicolae Filipoiu[1,2], and George Alexandru Nemnes[1,2,3] — [1]Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Magurele, Romania — [2]University of Bucharest, Faculty of Physics, 077125 Magurele-Ilfov, Romania — [3]Research Institute of the University of Bucharest (ICUB), Sos. Panduri 90, Bucharest Romania.

The problem of correctly identifying the biomarkers associated with specific pathologies is of great interest nowadays for rapid diagnoses. The transport properties of different active layers like beta-arsenate, phosphorene, graphene, or Al-doped MoSe2 were investigated in the presence of certain biomolecules. Additionally, predictions of biomolecular compounds with tunable gaps were reported as well as carbon nanotube-based. Our study brings a detailed analysis of 2D semiconductor heterostructures in contact with biomarkers of respiratory diseases, which exhibit large tunabilities in transport properties. As a first step, by using DFT simulations, the electronic properties of the systems are analyzed under different doping conditions and nanostructuring. In a second step, a large number of systems will be considered

for transport calculations and the results will define the input for machine learning procedures. This involves the mapping between structural information and transport properties. In the end, an analysis of the sensor's limit of detection and regeneration is performed.

DS 12.44 Wed 17:00 P3

Microstructure investigation of pulsed laser deposited GeTe-Sb_2Te_3 heterostructures — •Sonja Cremer[1], Lennart Voss[2], Nils Braun[1], Lorenz Kienle[2], and Andriy Lotnyk[1,3,4] — [1]Leibniz Institute of Surface Engineering, Leipzig — [2]Faculty of Engineering, University of Kiel — [3]Laboratory of Infrared Materials and Devices, Ningbo University — [4]College of Physics and Optoelectronic Engineering, Harbin Engineering University

Heterostructured phase change materials are an auspicious candidate to overcome high power consumption and resistance drift, hindering the implementation of Ge-Sb-Te based thin films for neuromorphic computing. Aiming at future systematic performance improvement, the impact of deposition parameters on the microstructure of GeTe-Sb_2Te_3 heterostructures (HSs) was investigated. HSs were grown at RT onto SiO_2/Si by PLD. Combining advanced TEM with XRD the microstructure was investigated in-depth. Energy and number of laser pulses affect the layer thickness and composition. The low energy and number of pulses lead to pronounced intermixing and hence to the formation of a single $GeSb_2Te_4$ layer. Besides, the local structure of the layers within the HS differs. While GeTe layers are amorphous, Sb_2Te_3 layers are polycrystalline and contain nanocrystals featured by varying sizes, defects and multiple phases. Thus, deposition parameters mainly affect the morphology and chemical composition of GeTe-Sb_2Te_3 HSs. However, the main factor influencing the crystallinity of the HS layers is the alloy itself. Financial support by the DFG (No. 445693080) is acknowledged. We thank A. Mill for assistance in FIB preparation.

DS 12.45 Wed 17:00 P3

Dynamics of ion beam-induced defects in phase-change materials investigated by in-situ optical measurements — •Sebastian Gratz, Marcel Buch, Martin Hafermann, and Carsten Ronning — Institute of Solid State Physics, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

Phase-change materials (PCMs) provide the ability of reversible, repeatable and rapid switching between amorphous and crystalline states. These transformations are accompanied with drastic changes of the electrical and optical properties, which is already been used in rewritable optical data storage or phase-change electronic memory. The transitions can be triggered by external thermal, optical, or electrical stimuli. The most extensively studied PCMs are pseudo-binary $(GeTe)_m(Sb_2Te_3)_n$ chalcogenide compounds (m, n being integer values), short GST. Ion irradiation was recently introduced to induce structural disorder and amorphize initially crystalline GST films. There are multiple studies that investigated the effect of defect engineering of GST compounds. However, there is still a lack of understanding of the dynamic effects, such as dynamic annealing of defects during the ion irradiation process. Furthermore, the direct impact of the specific GST stoichiometry on the ion-beam induced disorder has not been observed yet. Thus, we investigated the dynamics of defect formation for different GST stoichiometries, such as $Ge_1Sb_2Te_4$ (m=1, n=1), $Ge_1Sb_4Te_7$ (m=1, n=2), and $Ge_2Sb_2Te_5$ (m=2, n=1), via in-situ optical measurements during ion irradiation at different temperatures.

DS 12.46 Wed 17:00 P3

Preparation and characterization of Cu-Te phases using focused ion beam — •Nils Braun[1], Vladimir Roddatis[2], Agnes Mill[1], Sonja Cremer[1], Hagen Bryja[1], Lennart Voss[3], Lorenz Kienle[3], and Andriy Lotnyk[1,4,5] — [1]Leibniz Institute of Surface Engineering e.V. (IOM) — [2]GFZ German Research Centre for Geosciences — [3]Institute for Materials Science, Faculty of Engineering, University of Kiel — [4]Laboratory of Infrared Materials and Devices, The Research Institute of Advanced Technologies, Ningbo University — [5]College of Physics and Optoelectronic Engineering, Harbin Engineering University

In this work, we prepared different nanoscale Cu-Te phases from Cu - Sb_2Te_3 system using FIB. Copper chalcogenides have shown promising thermoelectric properties, e.g. high efficiency and tunability. Sb_2Te_3 thin layers are epitaxially grown on p-type Si (111) substrates and polycrystalline Sb_2Te_3 thin film are grown on a SiO_2 coated wafer using PLD. A standard cross-section FIB preparation method is used. Samples are investigated using advanced TEM methods and XRD. Dependent on beam current used during FIB lamella preparation and Sb_2Te_3 layer thickness, hole formation in the Cu layer, thickness change and chemical changes of the Sb_2Te_3 layers are observed. In specimen prepared from the heated samples Sb_2Te_3 and Cu-Te grains are found. In polycrystalline Sb_2Te_3 specimen the intercalation of Cu and formation of new Cu-Te phases is observed. We thank P. Hertel for magnetron sputtering. We acknowledge the financial support by the German Research Foundation (DFG 448667535).

DS 12.47 Wed 17:00 P3

Investigation of the insights of a TiN-PEALD process in a remote capacitively coupled plasma ALD reactor — •Jan Biedinger, Jan-Michael Schmalhorst, and Günter Reiss — Bielefeld University, Faculty of Physics, Germany

Atomic Layer Deposition (ALD) is a deposition technique of great interest due to precise and reproducible layer control, large-area uniformity and conformal coating. As it bases on chemical surface reactions, it is important to understand the mechanism of an ALD process. In the presented study, the effect of different process parameters (temperature, plasma power, plasma pulse length, NH_3 flow, plasma pressure) was studied in a titaniumnitride (TiN) plasma-enhanced ALD process, consisting of sequential pulsing of tetrakis(dimethylamido)titanium (TDMAT) and a NH_3 plasma. X-ray reflectivity and 4-point probe measurements were performed to determine the growth rate, roughness, density and electrical resistivity of all TiN films, respectively. Additionally, Auger electron spectroscopy revealed information about the chemical composition. By combining in-situ mass spectrometry data, where plasma species as well as reaction products could be identified during the process, with these ex-situ results, the process could be described in more detail. During the NH_3 step, the release of dimethylamine groups was observed, which decreased gradually with time. This correlates with the decline of carbon content by increasing the NH_3 step time. Moreover, it was observed that the plasma species (hydrogen and nitrogen radicals) seems to be responsible for decreasing the oxygen content and hence, improving thin film quality.

DS 12.48 Wed 17:00 P3

Epitaxial growth of $Ag_xCu_{1-x}I$ on Al_2O_3 (0001) — •E. Krüger[1], V. Gottschalch[2], G. Benndorf[1], R. Hildebrandt[1], A.L. Pereira[1], M. Bar[1], E. Abo El Fadl[1], S. Blaurock[2], S. Merker[2], C. Sturm[1], M. Grundmann[1], and H. Krautscheid[2] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper iodide (CuI) and related alloy compounds are of great interest as suitable materials for applications in fully transparent optoelectronic devices. While CuI exhibits intrinsic p-type conductivity with excessive high hole densities typically around $10^{18} - 10^{19}$ cm^{-3}, it was recently shown that the carrier density can be strongly reduced for $Ag_xCu_{1-x}I$ alloy and even n-type conductivity can be achieved for high Ag contents [1]. Here we present the epitaxial growth of $Ag_xCu_{1-x}I$ thin films on Al_2O_3 (0001) substrates using sublimation technique [2]. We demonstrate that $Ag_xCu_{1-x}I$ thin films with $x \leq 0.5$ exclusively exhibit the zincblende γ-phase, while a coexistence of zincblende γ- and wurtzite β-phases is observed for Ag-rich alloy compositions. In addition we provide the epitaxial relationships between the different $Ag_xCu_{1-x}I$ phases and the Al_2O_3 substrate. Moreover, we present another deposition approach based on a solid-state reaction between CuI and AgI, which allows the preparation of single-phase γ-$Ag_xCu_{1-x}I$ films up to $x = 0.7$.

[1] A. Annadi and H. Gong, Appl. Mater. Today **20**, 100703 (2020)
[2] E. Krüger et al., Phys. Stat. Solidi B (accepted)

DS 12.49 Wed 17:00 P3

Growth of CoO Thin Films for Application in Superconductor - Magnet Heterostructures — •Amy McGlinchey — Trinity College Dublin, Ireland

Cobalt monoxide, CoO, is an antiferromagnet (AF) with a Néel temperature of 293K. It is utilised to pin the magnetisation of Co layers via exchange bias and is employed in magnetic heterostructures. The interaction between ferromagnet (F) and AF layers is predicted to generate long-range spin-triplet superconductivity in F-S-AF heterostructures [1]. CoO is a good candidate for the AF due to its low Néel temperature, which facilitates in-field cooling through the transition improving magnetic homogeneity. For the most part, CoO is synthesized by the oxidation of Co thin films or using techniques such as spray pyrolysis and pulsed laser deposition. In this work, we focus on

the growth of CoO by molecular beam epitaxy, investigating the crystalline quality of the CoO as a function of deposition conditions. We have optimised these conditions to grow single crystalline CoO(100) thin films on MgO(100) substrates. As a second step towards a F-S-AF heterostructure, we also investigate the superconducting properties of Nb grown on CoO films. Due to the proximity effect, the properties of the niobium - especially at low thickness relevant to heterostructures - will be influenced by the CoO magnetic and interface structure [2]. 1. L. G. Johnsen et al., Phys. Rev. B, 103, L060505 (2021). 2. G. A. Bobkov et al., Phys. Rev. B, 106, 144512 (2022).

DS 12.50 Wed 17:00 P3

Potential of La-doped SrTiO3 thin films grown by metal-organic vapor phase epitaxy for thermoelectric applications — •Mohamed Abdeldayem[1], Aykut Baki[1], Carlos Morales Sánchez[3], Jan Ingo Flege[3], Detlef Klimm[1], Andreas Fiedler[1], Oliver Bierwagen[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institut für Kristallzüchtung, Berlin, Germany — [2]Paul Drude Institut für Festkörperelektronik, Berlin, Germany — [3]Brandenburgische Technische Universität Cottbus, Brandenburg, Germany

Conversion of waste heat energy into electrical energy by exploiting the thermoelectric effect in solids promises a great contribution to energy harvesting concepts. However, most thermoelectric materials use toxic Pb or Te. Recently, La-doped SrTiO3 has gained a lot of interest as a potential candidate for thermoelectric devices for its good thermoelectric properties, chemical and thermal stability. In this paper, we report the homoepitaxial growth of La-doped SrTiO3 thin films by metalorganic vapor phase epitaxy (MOVPE) technique, which works at high oxygen partial pressures and offers upscaling potential for industry. The adjustment of charge carrier concentration, necessary for thermoelectric power factor optimization, was performed by introducing a defined amount of the metal-organic precursor La(tmhd)3 and tetraglyme to the liquid precursor solution. X-ray diffraction and atomic force microscopy verified a pure perovskite phase with high structural quality. The electrical conductivity increases linearly with the La concentration in the gas phase, which is attributed to the substitution of La+3 ions on the Sr+2 sites inferred from photoemission spectroscopy.

DS 12.51 Wed 17:00 P3

Ultrathin alumina membrane: A new opportunity for constructing stable sodium metal anodes — •Jiajia Qiu, Changfan Xu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Unstable solid electrolyte interphase (SEI) remains a major bottleneck for sodium metal batteries due to the mossy or dendritic growth of Na in the repetitive stripping/plating process. Recently, nanostructured modification of Na and Al2O3 coatings have been reported as two effective solutions to address this issue. Accordingly, with almost identical pore regularity and precisely controlled geometrical structure, ultrathin alumina membrane (UTAM) is utilized as a functional layer to effectively protect the Na anode of Na-metal batteries for the first time in this work. The mossy or dendritic growth of Na has been suppressed due to the UTAM protection, resulting in a uniform electrodeposition interface. UTAM significantly improved the Coulombic efficiency while avoiding short circuit risks. And it has the potential to be applied to other metal anodes. The novel design of a UTAM-protected metal Na anode may bring in new opportunities for next-generation high performance Na metal batteries.

DS 12.52 Wed 17:00 P3

Contact printed micro circuit boards for thermoelectric circuits in van der Waals high temperature twisted cuprate heterostructures — •Sanaz Shokri[1,2], Christian N Saggau[1], Kornelius Nielsch[1,2], and Nicola Poccia[1] — [1]Institute for Metallic Materials, IFW Dresden, Dresden,Germany, IFW Dresden — [2]Institute for Materials Science, Dresden University of Technology

Recently, thermoelectric measurement has been established as an indicator of the topological nature of material due to its sensitivity to the Berry curvature. Nernst effect, which is defined as a generation of transverse electric field by a longitudinal temperature gradient in the presence of a magnetic field, in particular, is a powerful tool to investigate the area above superconductivity transition temperature where the transverse electrical signals become very small. Twisted Bi2Sr2CaCu2O8+δ (BSCCO) van der Waals heterostructures have exhibited topological superconductivity. Nevertheless, the BSCCO is too fragile to make a complex circuit like thermoelectric. Therefore, we developed the whole thermoelectric circuit like Seebeck and Nernst, embedded within inorganic SiN so called nanomembrane and transferred it on the optimally doped BSCCO flake inside the Ar-filled glovebox to encapsulate the BSCCO flakes and contact it at the same time. We used Pt as a heater and gold as the thermocouples and will calibrate our measurements based on the heat losses through a thermal insulating substrate and nanomembrane as well.

DS 12.53 Wed 17:00 P3

Preparation and characterization of Zn1-xMgxO thin films obtained by the aerosol deposition method for UV radiation detector — •Vadim Morari — Techical University of Moldova, D. Ghitu Institute of Electronic Engineering and Nanotechnologies, Chisinau, Republic of Moldova

Zn1-xMgxO ternary oxide solutions with wide band gap were prepared by the aerosol spray deposition method [1] using zinc acetate and magnesium acetate as precursors. This technique offers the possibility of rapid deposition of homogeneous thin films with good electrical and optical properties. It is suitable for growing high-quality thin films on Si, quartz, glass or sapphire substrate, with relatively large areas at low cost due to vacuum-free equipment, low temperatures during deposition, low defect density and low environmental impact. The obtained thin films were characterized by scanning electron microscopy (SEM), energy dispersive X-Ray analysis (EDX), X-Ray Diffraction (XRD), Raman spectroscopy and optical absorption spectroscopy. The investigation of photosensitivity revealed that multilayer ZnMgO structures with different Mg content are more sensitive than single-layer films in a wide spectral range from visible to the ultraviolet (UV-C) radiation.

[1] Morari,V., et. All. Photosensivity of heterostructures produced by aerosol deposition of ZnMgO thin films on Si substrates. In: Proceedings of SPIE - The International Society for Optical Engineering, vol. 11718, p. 1171818:1*8, (2020). https://doi.org/10.1117/12.2571189.

DS 12.54 Wed 17:00 P3

Heterostructure diodes based on reactively co-sputtered $Ag_xCu_{1-x}I$ thin films — •Jorrit Bredow, Sofie Vogt, Christiane Dethloff, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Germany

Copper iodide (CuI) is a transparent p-type semiconductor that exhibits high hole mobilities of up to 25 cm^2/Vs in polycrystalline thin films[1]. This renderes CuI an interesting candidate for the fabrication of transparent heterostructure diodes, such as p-CuI/n-ZnO[2], or p-CuI/n-AgI[3]. CuI further exhibits a low resistivity, which was shown to be increased with an increasing fraction of silver (Ag) in $Ag_xCu_{1-x}I$ thin films[4]. Moreover, a transition from p-type to n-type material of the $Ag_xCu_{1-x}I$ thin films for $x \approx 0.5$ was observed[4]. However, the $Ag_xCu_{1-x}I$ thin films were prepared with the Bädeker method, i.e. the iodization of metallic Ag_xCu_{1-x} thin films.

We present transparent heterostructure diodes based on the ternary compound $Ag_xCu_{1-x}I$. The $Ag_xCu_{1-x}I$ thin films were deposited using reactive co-sputtering of metallic Cu and Ag in Ar and I atmosphere. The feasibility of pn-heterojunction diodes with varying silver content is presented.

[1] C. Yang *et al.*, ACS Appl. Electr. Mater., 2, 3627-3632, 2020.
[2] F.-L. Schein *et al.*, Appl. Phys. Lett., 102, 092109, 2013.
[3] J.-H. Cha and D.-Y. Jung, ACS Appl. Mater. Interfaces, 9, 43807-43813, 2017.
[4] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.

DS 12.55 Wed 17:00 P3

SnTe topological insulator thin film for field-effect transistors — •Sepideh Izadi, Negin Beryani Nezafat, and Gabi Schierning — Department of physics, Experimental physics, Bielefeld University, 33615, Bielefeld, Germany

Topological insulators (TIs) as a new class of quantum materials are one of the potential interests for device fabrication. The unique electrical characteristics of TIs arises from robust metallic states passing through the bulk semiconducting band gap within the material. These surface states with high electrical mobility are considered as an efficient factor regarding high performance transistor. We herein present SnTe topological insulator as a potential candidate for active layer in field-effect transistor (FET). In this work the results of SnTe transistor device fabrication is reported using bottom gate approach. Therewith, Si3N4 and Al2O3 are applied as gate insulating material which are deposited using magnetron sputtering and atomic layer deposition (ALD), respectively. The provided findings and analysis in this work

paves the way for SnTe electrical device characterization.

DS 12.56 Wed 17:00 P3

Electric field induced laser-assisted polarization switching dynamics in ferroelectric thin films — •Rekikua Sahilu Alemayehu[1], Matthias Rössle[2], and Matias Bagrheer[1,2] — [1]Institute for Physics & Astronomy, University of Potsdam, Karl-Liebknecht-Str 24-25, 14476 Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Nucleation and growth of domains with opposite polarization moderates the electric field-induced polarization reversal process in ferroelectric materials. Accordingly, the domain wall velocity governs the timescale of polarization switching. Achieving the ultimate switching time in ferroelectrics is a fundamental quest to improve the device response time. Here we show laser-assisted polarization switching dynamics in metal-ferroelectric-metal heterostructure via heat and strain waves induced by a femtosecond laser pulse.

DS 12.57 Wed 17:00 P3

Engineering Vertical Memristive Devices with TMDC Thin Films — •Anna Linkenheil[1,2], Theresa Scheler[3,2], Ole Gronenberg[4], Hendrik Gross[4], Michaela Blum[3,2], Tzvetan Ivanov[1,2], Benjamin Spetzler[1], Frank Schwierz[1], Peter Schaaf[3,2], Lorenz Kienle[4], and Martin Ziegler[1,2] — [1]Micro- and Nanoelectronic Systems, Faculty of Electrical Engineering and Information Technology, TU Ilmenau, Ilmenau, Germany — [2]Institute of Micro- and Nanotechnologies, MacroNano®, TU Ilmenau, Ilmenau, Germany — [3]Materials for Electrical Engineering and Electronics, Faculty of Electrical Engineering and Information Technology, TU Ilmenau, Ilmenau, Germany — [4]Synthesis and Real Structure, Faculty of Engineering, Kiel University, Kiel, Germany

Transition metal dichalcogenides (TMDCs) represent a class of promising materials for memristive devices, which become increasingly important for emerging information processing approaches. In particular, homogeneous thin-films of few layers thickness have advantageous properties for memristive devices, such as excellent scaling behavior combined with the potential integration into planar wafer technology. Here, we assess the electrical properties of sputtered MoS_2 based devices and analyze the material. The devices were fabricated in a 4-inch wafer thin film technology, allowing for a systematic electrical investigation. Various electrode materials as well as oxidation treatments and their respective influences on device performance are evaluated using Transmission Electron Microscopy (TEM), revealing probable switching mechanisms and their origin.

DS 13: Optical Analysis of Thin Films I

Time: Thursday 9:30–11:00 Location: SCH A 316

Invited Talk DS 13.1 Thu 9:30 SCH A 316

Towards Catalytic Applications of Infrared Laser Polarimetry — •Andreas Furchner[1] and Karsten Hinrichs[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Division Energy and Information, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.

Infrared (IR) polarimetry and ellipsometry are well-established non-destructive spectroscopic techniques for studying the refractive and absorptive properties of thin films and surfaces with monolayer sensitivity. This spectral range is particularly suited for investigating chemical composition, molecular interactions, anisotropy, conductivity, as well as changes and reactions at surfaces and interfaces.

The incorporation of quantum cascade lasers (QCLs) in novel IR polarimeter designs has pushed the boundaries of the achievable spatial and temporal resolution well into the sub-mm and sub-second range, respectively. Laser-based polarimeters thus enable hyperspectral and time-resolved amplitude–phase measurements with novel application potential. Probing individual laser pulses delivers time resolutions of 10 μs, spectral sweeps in 100 ms, and hyperspectral maps in minutes.

This presentation focuses on recent instrumental developments, such as the combination of QCLs with single-shot designs, that pave the way towards the application of IR laser polarimetry in thin-film catalysis. Here, surface reactions have to be studied *in situ* and *operando* in order to resolve the evolution of surface species and temporary adsorbates.

DS 13.2 Thu 10:00 SCH A 316

Large area functional thin film properties mapping using in-line hyperspectral imaging during roll-to-roll magnetron sputter deposition — Florian Gruber[2], Patrick Schlenz[1], Steffen Bieder[4], Eric Schneider[4], Jolanta Szelwicka[1], Julio Hernandez[3], Christian Sternemann[4], and •Steffen Cornelius[1] — [1]Fraunhofer FEP, Winterbergstrasse 28, 01277 Dresden, Germany — [2]Fraunhofer IWS, Winterbergstrasse 28, 01277 Dresden, Germany — [3]Norsk Elektro Optikk AS, Ostensjoveien 34, 0667, Oslo, Norway — [4]Fakultät Physik/DELTA, Technische Universität Dortmund, August-Schmidt-Straße 1, 44227 Dortmund, Germany

Roll-to-roll (R2R) coating processes of flexible substrates are established for cost-efficient thin film functional materials production for applications like energy efficient windows and solar cells. However, even small variations of thickness and/or composition homogeneity may affect the final product performance. Due to the high throughput of coated surface area in R2R coating the ex-situ material characterization is very time consuming, often destructive and offers no possibility for in-situ process monitoring and/or quality control.

The NanoQI EU-H2020 project develops a powerful in-line technology combining hyperspectral imaging with X-ray reflectivity via a machine learning algorithms, enabling large area (0.5m x 100m) high resolution (<1mm) high speed (m/min) thin film properties imaging. The combinatorial thickness mapping of a binary metal-oxide double layer (thickness up to 120nm) on PET substrate will be discussed in detail - aiming to achieve a thickness accuracy of only a few %.

DS 13.3 Thu 10:15 SCH A 316

Developing an open source ellipsometry analysis workflow — •Florian Dobener[1], Marius Müller[2], Carola Emminger[1,3], Chris Sturm[3], Tamás Haraszti[4], Marius Grundmann[3], and Sandor Brockhauser[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Germany — [2]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [3]Felix-Bloch Institut für Festkörperphysik, Universität Leipzig, Germany — [4]DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Optical and geometric characteristics of multilayer material stacks are not accessible from ellipsometric data in a direct way. The optical model applied to the data is the key, which allows understanding of these properties. Accordingly, there exist a lot of different software tools to construct such models, which vary in their model implementation and are often closed source. Comparing, reproducing and using data from literature can therefore be challenging. Here, we present the open source ellipsometry software pyElli. It implements specific dispersion models from manufacturers and from literature. Furthermore, it allows for easy construction of non-standard measurement tasks, e.g. combining different measurements or using uncommon measurement parameters. Together with the recent NeXus ellipsometry standard, the NOMAD research data management platform and its interactive Jupyter based toolkit, we show how pyElli contributes to an open ellipsometry workflow. This open workflow is a standardised and reproducible way of analysing ellipsometry data and adds to the goal of making ellipsometry data FAIR.

DS 13.4 Thu 10:30 SCH A 316

IR dual-comb polarimetry of anisotropic nanofibers — •Karsten Hinrichs[1], Brianna Blevins[2], Andreas Furchner[3], Nataraja Sekhar Yadavalli[2], Sergiy Minko[2], Raphael Horvath[4], and Markus Mangold[4] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Department of Chemistry, The University of Georgia — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Division Energy and Information, Schwarzschildstraße 8, 12489 Berlin, Germany — [4]IRsweep AG, Laubisruetistrasse 44, 8712 Staefa, Switzerland

In this work an anisotropic nanofiber scaffold is investigated non-invasively under ambient conditions by infrared dual-comb polarimetry (IR - DCP). Amplitude and phase spectra at various azimuthal sample rotations are correlated with the orientation of characteristic

vibrational transition dipole moments. IR - DCP is proven as a new method for the spectral analysis (here 1200 cm-1 to 1300 cm-1) of such anisotropic samples in very short measurement times (0.065 ms) at 1.4 cm-1 spectral resolution. Such capabilities are in particular interesting for imaging applications, time resolved studies and hyperspectral spectroscopy of anisotropic samples. In difference to classical ellipsometry which measures phase differences, IR - DCP can measure s- and p-polarized phases separately. We acknowledge financial support by the EU through EFRE 1.8/13 and the Horizon 2020 grant 820419 and by the BMBF through CatLab (03EW0015A/B).

DS 13.5 Thu 10:45 SCH A 316

Orientation in thin spider silk films at silicon substrates evidenced by dichroic FTIR spectroscopy — •Martin Müller[1,2], Mirjam Hofmaier[1,3], Sarah Lentz[4], Thomas Scheibel[4], and Andreas Fery[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institut für Physikalische Chemie und Physik der Polymere, Dresden, Germany — [2]Technische Universität Dresden, Lehrstuhl für Makromolekulare Chemie, Dresden, Germany — [3]Technische Universität Dresden, Lehrstuhl für Physikalische Chemie Polymerer Materialien, Dresden, Germany — [4]Universität Bayreuth, Lehrstuhl für Biomaterialien, Bayreuth, Germany

Biomedically relevant spider silk films were deposited on unscratched and parallelly scratched silicon substrates and checked for conformation and orientation by dichroic transmission (T-) and ATR-FTIR spectroscopy. Films (d=0-200 nm) were casted from hexafluoroisopropanol solutions of recombinantly engineered spider silk proteins. Both FTIR methods revealed little b-sheet (<10%) and much disordered structure (>80%) from Amide I band analysis. Dichroic ratios R of Amide I components close to isotropic films were found by T- and ATR-FTIR indicating no orientation. Whereas, silk films after swelling in MeOH vapor revealed higher b-sheet (>30%) and lower disordered structure amounts (<60%). By T-FTIR isotropic R values of Amide I components assigned to antiparallel b-sheet were found indicating no in-plane orientation, while ATR-FTIR revealed R values significantly deviating from isotropy indicating out-of-plane orientation. Orientation was independent on scratching and increased decreasing d.

DS 14: Thin Oxides and Oxide Layers

Time: Thursday 9:30–11:15 Location: SCH A 315

DS 14.1 Thu 9:30 SCH A 315

Strain effects of the electronic and magnetic properties of thulium iron garnet films — •Sibylle Gemming[1], Georgeta Salvan[1], Apoorva Sharma[1], Oana T. Ciubotariu[2], and Manfred Albrecht[2] — [1]Institute of Physics, TU Chemnitz — [2]Institute of Physics, U Augsburg.

Rare earth iron garnets are magnetic insulators, in which two structurally distinct iron centers form sublattices, which couple antiferromagnetically. The overall magnetization of the compounds results from the alignment of the local magnetic moments of the 4f electrons at the rare earth sites and is sensitive to external effects such as temperature and strain. We performed gradient-corrected density-functional calculations including spin-orbit and correlation corrections to study the property-thickness relation of thin thulium iron garnet films that had been grown epitaxially under tensile strain on a doped gallium gadolinium garnet substrate. We could rationalize the observed growth modes for different film thicknesses with strain arguments and correlate it with the observed electronic properties (Funding: DFG, GE 1202/12-1)

DS 14.2 Thu 9:45 SCH A 315

Optoelectronic Properties of Al-doped ZnO Films Prepared by ALD and Flash Lamp Annealing — •Guoxiu Zhang[1,2], Oliver Steuer[1], Yu Cheng[1], Yi Li[1], Kaiman Lin[1], Shengqing Zhou[1], Yufei Liu[2,3], and Slawomir Prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, Dresden, 01328, Germany — [2]Key Laboratory of Optoelectronic Technology & Systems (Chongqing University), Ministry of Education, Chongqing 400044, China — [3]Faculty of Science and Engineering, Swansea University, Swansea SA2 8PP, UK

Zinc oxide (ZnO) is a wide-band-gap semiconductor considered for transparent and flexible optoelectronics. Effective and controlled doping of ZnO can be realized by substitution Zn or O atoms with metal or non-metal elements like H, Al, Ga for n-type doping and e.g. group V elements for p-type doping. In this work, we have investigated the optoelectronic properties of *-doped ZnO with Al. 100 nm thick Al-doped ZnO (AZO) films were deposited on Si wafers by atomic layer deposition (ALD) varying the distance between Al-layers. After ALD process samples were annealed using ms-range flash lamp annealing (FLA) in either nitrogen or oxygen atmosphere. The highest carrier concentration estimated from Hall-effect measurements is 2.7 *1021 cm-3 and the resistivity is 8.8*10-4 Ωcm, for AZO films where the Al-*-layer is separated by 20-layers of Zn. In general annealing in N2 atmosphere promotes n-type doping while annealing in O2 leads to the formation of highly resistive films.

DS 14.3 Thu 10:00 SCH A 315

Strain Engineering of Buffer Layers: A Way to Overcome Film/Substrate Lattice Misfit — •Pia Henning[1], Ulrich Ross[2], Karen Stroh[1], Vitaly Bruchmann-Bamberg[1], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

A fundamental problem in thin film physics is the film/substrate lattice misfit and the related epitaxial strain. An especially important role plays stress for perovskite manganites, e.g. colossal magnetoresistive $(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3$ (LPCMO), yielding a suppression of the metal-insulator and ferromagnetic phase transition for LPCMO thin films grown on standard perovskite substrates, like SrTiO3 (STO, tensile stress) and LaAlO3 (LAO, compressive stress). We propose a route to engineer the strain via LAO buffers epitaxially grown on STO substrates by means of metalorganic aerosol deposition to obtain epitaxial stress-free LPCMO films. By changing the LAO thickness in the range d_{LAO}∼2-35 nm and precisely tuning the stress in it, an ideal lattice adjustment between LPCMO and LAO has been achieved. This allows us to grow stress-free epitaxial LPCMO/LAO/STO(100) thin and ultrathin (d_{LPCMO}∼10 nm) films with bulk properties. The structure and microstructure of these films as well as the stress distribution within layers was studied by X-ray diffraction and high resolution transmission electron microscopy. A generalization of this method on other film/buffer/substrate combinations has been proposed.

DS 14.4 Thu 10:15 SCH A 315

Transfer and Thermal Processing of Freestanding Oxide Membranes — •Yu-Jung Wu, Varun Harbola, Sander Smink, Sarah C. Parks, and Jochen Mannhart — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Epitaxial films of complex oxides have gained interest due to their wide-ranging physical properties, including high-temperature superconductivity, magnetism, ferroelectricity, and multiferroicity. The conventionally grown single-crystalline oxide thin films are usually bound to their substrates, which imposes constraints on their properties and usage. Therefore, growth techniques have recently been developed that enable lifting-off freestanding complex oxide membranes by wet etching of oxide buffer layers. To achieve transfer of large-area oxide films, we have systematically studied growth and transfer of a variety of thin films, grown on aluminate and manganite wet-etchable buffer layers. Various oxide membranes were successfully transferred with good quality and up to 3x 2 mm2 area with minimal cracking. Furthermore, after thermal processing the stack of the transferred membrane on sapphire, the transferred membrane starts dewetting, yielding nanostructures. This work is not only expected to enable a wide range of oxide films to be transferred in high quality for fundamental studies and applications in oxide electronic devices but also serves as a starting point for crystalline nano-structuring of oxide materials.

DS 14.5 Thu 10:30 SCH A 315

Tungsten-oxide thin films characterized by Positron Annihilation Spectroscopy — •Vassily Vadimovitch Burwitz[1], Annemarie Kärcher[2,3], Lucian Mathes[1], Thomas Schwarz-

Selinger[3], Maik Butterling[4], Eric Hirschmann[4], Maciej Oskar Liedke[4], Andreas Wagner[4], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]TU München — [3]Max-Planck-Institut für Plasmaphysik, Garching bei München — [4]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

For future nuclear fusion reactors it is foreseen that tungsten is used as inner wall cladding. Understanding the formation and behaviour of radiation induced defects in tungsten is therefore important for their safe operation. Tungsten mono-crystal model systems are studied by positron annihilation Doppler-broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS) to foster the understanding of the type and evolution of these defects. Both methods are sensitive tools when examining the defect type and concentration. However, data obtained by either of these methods is influenced by any thin oxide film on the surface of a sample. Such a film is present on any tungsten sample exposed to air, therefore its effect on DBS and PALS results needs to be known for their correct interpretation. In this work we measured tungsten-oxide thin films grown by thermal and electrochemical methods as well as by exposure to air by DBS and PALS. The DBS measurements were performed using a moderated β^+ emitter, the PALS measurements at an accelerator-based positron source.

DS 14.6 Thu 10:45 SCH A 315

Monitoring switching process in Fe_3O_4/STO heterostructures via in-situ instrument — •Yifan Xu[1], Mai Hussein Hamed[1,2], Connie Bednarski-Meinke[1], Asmaa Qdemat[1], Steffen Tober[1], Emmanuel Kentzinger[1], Oleg Petracic[1], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Faculty of Science, Helwan University, 11795 Cairo, Egyp

The ability to tune magnetic oxide phases via redox reactions across their heterointerfaces could lead to useful spintronic and memristive device applications. By applying a small electric field, oxidation/reduction occurs at the heterointerface and leads to a reversible phase transition. In this talk, we present the preparation and characterization of epitaxial Fe_3O_4 thin films grown on TiO_2-terminated Nb:STO via pulsed laser deposition (PLD). Using magnetometry, we detect the Verwey transition; a strong indicator of the oxygen content in the Fe_3O_4 films. We observe the disappearance in the Verwey transition temperature with an applied positive electric field. This could be explained by oxygen diffusion through the interface which then leads to a reversible phase transition from Fe_3O_4(magnetite) to γ-Fe_2O_3(maghemite). Using ex-situ x-ray diffraction (XRD), we observe the structural transitions from (001) to (111) in the out-of-plane direction influenced by the applied voltage. Interestingly, by grazing-incidence small-angle X-ray scattering, we observe a change in the magnetite domain size for the sample after applying the electric field.

DS 14.7 Thu 11:00 SCH A 315

Engineering magnetic anisotropy by Rashba spin-orbit coupling in 3d-5d oxide heterostructures — •Megha Vagadia, Jaya Prakash Sahoo, Ankit Kumar, Suman Sardar, Tejas Tank, and D.S. Rana — 1Department of Physics, Indian Institute of Science Education and Research Bhopal, M.P. 462066, India

In recent times, Rashba spin-orbit coupling (SOC) has been successfully employed for the emergence of exotic phenomena at the quantum oxide interfaces. In these systems, the combined effect of charge transfer, broken symmetries, and SOC yields intriguing interfacial magnetism and transport properties. However, role of Rashba SOC, particularly without applied bias, in modulating magnetic anisotropy of oxide heterostructures is unexplored. Here, we provide insight into tuning transport phenomena by the charge transfer driven Rashba SOC in CaMnO3/CaIrO3 heterostructures. Rashba SOC remarkably enhances the anomalous Hall conductivity and reconstructs the Berry curvature. From the anisotropy magnetoresistance measurements, we demonstrate that Rashba SOC is instrumental in tailoring magnetic anisotropy where magnetization easy-axis rotates from the out-of-plane direction to the in-plane direction. The ability to tune Rashba SOC and resulting competing magnetic anisotropies provides a route to manipulate electronic band structure for the origin of non-trivial spin texture useful for spin-orbitronics applications.

DS 15: Optical Analysis of Thin Films II

Time: Thursday 11:15–12:45 Location: SCH A 316

Invited Talk DS 15.1 Thu 11:15 SCH A 316

In-Situ Optical Investigation of Electrochemically Induced Conformational Changes at Solid Liquid Interfaces: A Source of new Electronic States — •Christoph Cobet — Linz School of Education, Center for Surface- and Nanoanalytics (ZONA), Johannes Kepler University, Altenbergerstr 69, A-4040, Linz, Austria

The electrical potential between an electrolyte and a solid electrode, whether it is a metal, semiconductor, polymer or a bio-membrane, could induce considerable changes in the conformational appearance. In biological systems such conformation changes are well-known e.g. as a control element for the chemistry on one or both sides of a membrane. In periodically ordered thin films or at surfaces, one can observe conformation changes at the atomic length scale which could induce new electronic properties. The interfacial electrical potential is in all cases a very versatile control element. On the one hand, it allows to change the chemical formation potential over a huge range which is otherwise only accessible for example by rather extreme temperature or pressure differences. On the other hand, it offers a very precise control of the thermodynamic equilibrium conditions. With the help of in-situ optical methods like spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS), we could study the interplay of the potential induced charge accumulation, the conformational changes and the evolution of (self) localized electronic states. The mechanisms will be discussed by two examples: The electrochemical doping and formation of polarons in polymers and the formation of surface quantum well states at a metal-electrolyte interface.

DS 15.2 Thu 11:45 SCH A 316

Singlet fission and triplet dynamics in pentacene embedded in a surface-anchored metal-organic framework — •Martin Richter[1], Zhiyun Xu[2], Philipp Ludwig[3], Pavel Kolesnichenko[1], Uwe Bunz[3], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie — [3]Organisch-Chemisches Institut, Universität Heidelberg

It has been observed, that the rate of singlet fission in pentacene and the lifetime of the generated triplets strongly depend on the molecular arrangement.[1]

Here, a cofacial orientation of pentacene molecules is achieved by embedding them in a surface anchored metal-organic framework (SURMOF). Transient absorption spectroscopy has been used to analyze the ultrafast dynamics as well as long lived states after photoexcitation. The observed difference absorption spectra indicate, that after the initial excitation a singlet excited state generates a correlated triplet pair within a few picoseconds that retains singlet character. Subsequent dynamics show the formation of a long-lived species (47us) with triplet character. This exceeds by far the observed lifetime of triplets generated in pentacene thin films (10ns) and may enhance triplet harvesting capabilities in photovoltaic devices.[2]

1.Lubert-Perquel, D., Nat Commun. 2018, 9, 4222
2.Poletayev, A.D., Adv. Mater. 2014, 26, 919-924

DS 15.3 Thu 12:00 SCH A 316

Birefringence of orthorhombic DyScO3: Towards a terahertz quarter-wave plate — •Jingwen Li, Chia-Jung Yang, Jannis Lehmann, Nives Strkalj, Morgan Trassin, Manfred Fiebig, and Shovon Pal — D-MATL, ETH Zurich, Switzerland

The energy scale of THz light corresponds to plenty of the fundamental collective excitations in materials, such as phonons, magnons, and heavy fermions. This makes THz light an ideal tool to investigate the low-energy excitations and non-equilibrium processes in solid-state systems. With the growing interest in studying the aforementioned collective phenomena, manipulating the polarization of THz light becomes necessary. However, prevailing THz waveplates, such as quarter-wave

plates (QWPs) for generating circularly polarized THz light, typically suffer from various problems, including bulky size, complex fabrication, or narrow working ranges. Here, we present a broadband THz QWP based on a 50-μm-thick (110)-cut orthorhombic $DyScO_3$ (DSO) crystal. We show a polarimetry measurement to verify the polarization of the output CP-THz light and prove that our DSO plate behaves like a QWP over a broad frequency range of 0.50-0.70 THz with a phase tolerance of ±3%. We believe that our results expand the choices of broadband THz QWPs, as well as the possibilities of simple and compact achromatic THz QWPs by combining DSO crystals. Most importantly, as a common substrate for growing various thin films, DSO shows its potential as a compact built-in broadband THz waveplate for thin film research with circularly polarized THz light. [1]

[1] Appl. Phys. Lett. **118**, 223506 (2021).

DS 15.4 Thu 12:15 SCH A 316

Temperature Dependence of Coherent Phonon Oscillations in Metavalently Bonded Solids — •Timo Veslin[1], Felix Hoff[1], Julian Mertens[1], Jonathan Frank[1], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]PGI 10 (Green IT), Forschungszentrum Jülich GmbH

Femtosecond optical pump probe measurements are carried out in order to detect changes in the reflectivity of the material response of MBE grown metavalently bonded (MVB) materials on sub-ps timescales. MVB differs significantly from metallic, ionic and covalent bonding. Examination of reflectivity changes due to the coherent phonon response provides insight into the ultrafast lattice dynamics and relaxation of MVB materials. To this end, the mechanism of displacive excitation of coherent phonons (DECP) is used to analyse the highly symmetric A1 modes. The material response consists of the ultrafast carrier excitation and a slower carrier relaxation together with a damped harmonic phonon oscillation measured in the transient reflectivity trace. The temperature dependence of the frequency, lifetime and oscillation amplitude of the coherent phonon A1 mode in Sb2Te3, GeTe and Bismuth will be presented. This allows to identify phonon coupling effects and dephasing mechanisms, as well as the temperature dependence of phonon frequencies. Furthermore, the results are supported by optical and structural data recorded at room temperature. These measurements will help to better understand the MVB mechanism which governs phase change materials.

DS 15.5 Thu 12:30 SCH A 316

Identification of different polymorphs of a zone-cast perylene diimide derivative with low-frequency Raman and infrared scanning near-field microscopy — •Nadine von Coelln, Christian Huck, Niklas Herrmann, Petra Tegeder, and Jana Zaumseil — Institute of Physical Chemistry, Heidelberg University, Germany

Small-molecule organic semiconductors are prone to form multiple thin film polymorphs. As their charge transport characteristics may vary substantially, effective and fast polymorph characterization techniques are necessary. Here, zone-cast films of perfluorobutyl dicyanoperylenecarboxydiimide (PDIF-CN_2) were studied with X-ray diffraction (XRD), confocal low-frequency Raman microscopy and infrared scanning near-field microscopy (IR-SNOM). Based on low-frequency Raman spectra and XRD, two different thin film polymorphs of PDIF-CN_2 were identified, which form depending on the solvents used for deposition. While confocal Raman microscopy is limited in the spatial resolution of areas, the near-field infrared technique (IR-SNOM) offers the unique possibility of both infrared microscopy and spectroscopy with a spatial resolution down to ∼10 nm. We demonstrate that it is possible to discriminate between neighboring crystalline regions of the two PDIF-CN_2 polymorphs by means of IR-SNOM using slight differences in IR absorption. As a non-destructive technique, IR-SNOM may even enable in-situ investigations of thin semiconducting films in functional devices.

DS 16: Thermoelectric and Phase Change Materials; Layer Deposition

Time: Thursday 11:30–13:00 Location: SCH A 315

DS 16.1 Thu 11:30 SCH A 315

A Multiscale Simulation Method for Deposition Processes: Micrometer-scale Off-Lattice Film Growth with Atomistic Precision — •Erik E. Lorenz[1] and Jörg Schuster[2,1] — [1]Center for Mikrotechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany

We present a multiscale method for the simulation of thin film deposition processes such as PVD, CVD and ALD. By combining Kinetic Monte Carlo (KMC) methods for adsorption event sampling and Molecular Dynamics (MD) for adsorption simulation and nanostructure relaxation with a graph-based triangulating bulk-surface representation, fast and efficient highly-parallel surface growth simulations are facilitated.

The enhancement of KMC-MD coupling with a graph-based bulk-surface representation enables efficient subdomain decompositions, bulk KMC event insertions and removals, and the robust and constant-time update of connected subdomain. Using the same graph structure, the effects of further computational improvements such as incident particle ray tracing, surface diffusion and limited KMC time warping are shown.

We demonstrate the growth of atomistic copper seed layers on a Tantalum substrate for micrometer-scale electronic devices in parallelized simulation runs saturating over 1000 CPU cores, and compare it to established methods.

DS 16.2 Thu 11:45 SCH A 315

Characterization and optimization of MgZnO thin films with steep lateral composition gradient — •Laurenz Thyen, Max Kneiss, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

The materials magnesium- and zinc-oxide have been widely investigated in the past. Corresponding step graded ternary alloy thin films of $Mg_xZn_{1-x}O$ have been of great interest [1]. Pulsed laser deposition (PLD) has been used to grow laterally and vertically graded thin films [2]. The precise control of chemical composition is of great importance for possible applications. Additionally, in the course of miniaturization of electrical devices like wavelength-selective multi-channel UV photodetectors, a well-defined steep slope of the material gradient will be beneficial [3,4].

In this contribution the properties of $Mg_xZn_{1-x}O$ thin films with lateral compositional gradient grown by pulsed laser deposition will be discussed. In order to obtain information about the material composition of the thin films, energy-dispersed X-ray spectroscopy, spatially resolved ellipsometry and micro-photoluminescence spectroscopy measurements have been conducted. Moreover, steep lateral gradients with a slope of up to 20 % Mg/mm were realised.

[1] Z. Zhang, *et al.* IEEE Journal Quantum Elec, 20.6, 106-111, (2014)
[2] H. v. Wenckstern, *et al.* physica status solidi (b) 257.7 (2020)
[3] M. Grundmann, IEEE Transact. Elec. Dev. 66.1 (2018): 470-477
[4] M. Kneiß, *et al.* ACS Combinatorial Science 20.11 (2018): 643-652.

DS 16.3 Thu 12:00 SCH A 315

Physical properties of $Ni_xCu_{1-x}I$ thin films deposited by magnetron co-sputtering — •Christiane Dethloff, Sofie Vogt, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institut, Universität Leipzig, Deutschland

The highly conductive, p-type semiconductor CuI is subject to various doping approaches to tailor optical and electrical properties [1-4]. As recently shown [5], doping CuI with Ni reduces its high hole density of up to 2×10^{19} cm^{-3} [4]. After surpassing a threshold of 15 % Ni content, a carrier conversion, as observed by Annadi *et al.*, turns the $Ni_xCu_{1-x}I$ alloy into an n-type semiconductor, which predestines $Ni_xCu_{1-x}I$ to fabricate p-n-homojunctions.

We present our investigations regarding morphology, electrical and possible ferromagnetic properties of $Ni_xCu_{1-x}I$ thin films with varying Ni contents. The deposition was conducted by reactive magnetron co-sputtering of metallic Cu and Ni in an iodine and argon athmosphere. X-ray and scanning electron microscope as well as Hall-effect and conductivity measurements were used to investigate the thin films. First

measurements yielded a low resistivity of 5×10^{-3} Ωm for x=0.035.

[1]T. Jun *et al.*, Advanced materials 2018 30, e1706573
[2]H. Wu *et al.*, Appl. Phys. Lett. 2021 118, 222107
[3]P. Storm *et al.*, Phys. Status Solidi RRL. 2021 15, 2100214
[4]A. Annadi *et al.*, Applied Materials Today. 2020 20, 100703
[5]A. Annadi *et al.*, ACS applied materials & interfaces. 2020 12, 6048

DS 16.4 Thu 12:15 SCH A 315

Self-assembled droplet etching during semiconductor epitaxy for versatile quantum structures — •Christian Heyn, Ahmed Alshaikh, and Robert Blick — Center for Hybrid Nanostructures (CHyN), University of Hamburg

As a fundamental extension of conventional epitaxy, we describe the integration of self-assembled top-down strategies into the bottom-up molecular beam epitaxy (MBE) of semiconductor quantum structures (QS). The samples are fabricated using standard solid-source MBE without any additional equipment. Ga, Al, or In droplets are formed on a GaAs or AlGaAs surface driven by the minimization of surface and interface energies in Volmer-Weber mode. The metal droplets drill self-assembled nanoholes into the semiconductor surface which is called local droplet etching (LDE). Afterwards, the nanoholes are filled with a material different from the substrate for the generation of QS. This presentation discusses the general mechanism of LDE, the influence of the process parameters on the density, size, and shape of the resulting nanoholes, as well as an intermixing with substrate material. For LDE with Ga droplets on AlGaAs, a crystalline wall formed around a nanohole represents a GaAs quantum ring. Further strain-free QS are created by filling of nanoholes drilled using Al droplets in AlGaAs with GaAs. The size and shape of the resulting QS is controlled by the initial nanohole, the amount of deposited material for hole filling, and capillary. Examples are QS that are shaped like the shell of a cone and vertically coupled quantum dot molecules.

DS 16.5 Thu 12:30 SCH A 315

Interplay of Glass Dynamics and Crystallization Kinetics of Photonic Phase Change Materials Sb2S3 & Sb2Se3 — •Felix Hoff[1], Julian Pries[1], Maximilian J. Müller[1], Eric N. Lensker[1], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]PGI 10 (Green IT), Forschungszentrum Jülich GmbH

Due to their large bandgaps, the chalcogenide phase-change materials (PCM) antimony sulfide Sb2S3 and antimony selenide Sb2Se3 are interesting for photonic applications in the visible and telecommunication wavelength range. They are promising for photonic integrated circuits or tunable metasurfaces. While recent literature focuses on the optical properties and the resulting applications, a systematic quantification of the amorphous glass phase, as well as its influence on the process of crystallization under different conditions, is missing. In this work, both the standard glass transition and fragility of antimony sulfide are presented and discussed. Sb2S3 is found to crystallize from the undercooled liquid phase for all technologically relevant heating rates spanning over six orders of magnitude. In contrast, Sb2Se3 appears to show a glass transition only for higher heating rates. This can be used to explain the unusual temperature dependence of its crystallization mechanism in thin films.

DS 16.6 Thu 12:45 SCH A 315

Seebeck coefficient inversion in highly doped organic semiconductors — •Morteza Shokrani[1], Kai Xu[2], Tero-Petri Ruoko[2], Dorothea Scheunemann[1], Hassan Abdalla[2], Hengda Sun[2], Chi-Yuan Yang[2], Yuttapoom Puttisong[2], Nagesh Kolhe[3], José Silvestre Mendoza Figueroa[2], Jonas Pedersen[2], Thomas Ederth[2], Weimin Chen[2], Magnus Berggren[2], Samson Jenekhe[3], Daniele Fazzi[4], Martijn Kemerink[1,2], and Simone Fabiano[2] — [1]Heidelberg University, Germany — [2]Linköping University, Sweden — [3]University of Washington, USA — [4]University of Cologne, Germany

The investigation of the thermoelectric properties of organic semiconductors (OSC) with the aim of increasing their efficiency as active material in thermoelectric generators has attracted attention for the past years. The maximum efficiency of the energy conversion process in a thermoelectric material is set by zT, which is proportional to electrical conductivity and Seebeck coefficient (S) squared. A common way of increasing zT is by doping, which typically increases the charge carrier density and electrical conductivity, while decreasing S. The sign of S is often used to determine the polarity of the majority charge carriers in OSC. In recent years, a surprising change in the sign of S has sometimes been observed to occur in highly doped OSC. Here, by combining conductivity and S measurements with kinetic Monte Carlo simulations, it is shown that density of state filling in combination with the opening of a hard Coulomb gap around the Fermi energy is responsible for the sign inversion

DS 17: Optical Analysis of Thin Films III

Time: Thursday 16:15–17:45 Location: SCH A 316

Invited Talk DS 17.1 Thu 16:15 SCH A 316

In-situ optical spectroscopy on electrochemical interfaces: From OER electrocatalysts to "smart" electro-switchable interfaces — •Martin Rabe — Department of Interface Chemistry and Surface Engineering, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

We employ electrochemical in-situ optical spectroscopies, namely IR- and Raman-spectroscopy as well as UV/vis-spectroscopic ellipsometry to understand fundamental processes at electrolyte/solid interfaces. Here, different examples from our research will be presented and discussed. 1: Electrocatalytically active manganese and nickel oxides during the anodic oxygen evolution reaction (OER) were studied. The formation, phase transitions and dissolution processes in these metal oxides is shown to govern their activity and stabilities on metallic electrodes. These material properties play a major role for the improvement of electrocatalysts for the sluggish OER in hydrogen production by the electrochemical water splitting. 2: The impact of the electrochemical Ge-OH to Ge-H surface termination on germanium interfaces was studied, which is accompanied by a switching of the interface hydrophobicity. The formation of a hydrophobic gap at semiconductor/electrolyte interface gives access to study fundamental properties of the water solvation layers. Furthermore, it is shown how the macroscopic change of the hydrophobicity can be employed as a "smart" electro-switchable surface that allows to reversibly control the adsorption and orientation of bio-macromolecules, a process that is potentially useful for novel bio sensing applications.

Invited Talk DS 17.2 Thu 16:45 SCH A 316

The physics of low symmetry semiconductors: Gallium oxide for the future of green energy as example — •Mathias Schubert — Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA — NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden

The physics of Gallium arsenide (zincblende structure) and Gallium nitride (wurtzite structure) led to disruptive technologies driven by extreme properties such as small effective mass, large direct bandgap, and piezoelectric polarization. Gallium reappears in a monoclinic crystal structure Oxide with enormous prospects for applications in power electronics for the future of green energy. Numerous new phenomena hitherto unknown for traditional semiconductors occur in monoclinic symmetry semiconductors such as non-parallel phonon-plasmon scattering, hyperbolic shear polaritons, splitting of associated transverse and longitudinal phonon modes, non-degenerate highly anisotropic fundamental excitonic band-to-band transitions, directional band offsets, and complex defect spin interactions within the highly anisotropic host lattice. The influences of composition, strain, doping, and defects are discussed for Gallium oxide and related alloys, and special emphasis is given to new semiconductor physics, and consequences for thin film growth and device designs are pointed out. Methods such as generalized ellipsometry, the optical Hall effect, Terahertz electron paramagnetic resonance ellipsometry, and density functional perturbation theory computations are employed for characterization and analysis.

Invited Talk DS 17.3 Thu 17:15 SCH A 316

Spectroscopic ellipsometry studies of optical constants in highly excited semiconductors — •Stefan Zollner — New Mex-

ico State University, Las Cruces, NM, USA

Spectroscopic ellipsometry is an optical reflection technique with polarized light. Most commonly, it is used to measure the thicknesses of thin-film layers, such as SiO_2 on Si. But it can also be used to study the energies and broadenings of elementary excitations in solids, such as electrons (band gaps, transport), infrared active phonons, and their interactions. We previously reported precision measurements of the complex refractive index of germanium near the direct band gap, which allowed us to compare our results quantitatively with theoretical predictions from Fermi's Golden Rule, based on k.p theory and including the excitonic interaction between electrons and holes. Going further, we can investigate how many-body effects impact the properties of electrons in highly excited semiconductors. Large carrier concentrations can be achieved through doping, thermal excitation of electron-hole pairs in small band-gap semiconductors, or optical excitation with ultrafast lasers. In this talk, I will report recent ellipsometry results for the temperature-dependent dielectric function of InSb near the direct band gap and the transient dielectric function of Ge near the E_1 and $E_1 + \Delta_1$ transitions from femtosecond pump-probe ellipsometry. I will also point out the theoretical approach needed to explain these data sets.

DS 18: Members' Assembly

Time: Thursday 18:00–19:00 Location: SCH A 315

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