Thin Films Division
Fachverband Dünne Schichten (DS)

Stefan Krischok
Technische Universität Ilmenau
Weimarer Straße 32
98693 Ilmenau
stefan.krischok@tu-ilmenau.de

Overview of Invited Talks and Sessions

(Lecture halls A 053 and A 060; Poster B and D)

Invited Talks

DS 3.1	Mon	15:00–15:30	A 053	**Advances in AlN-based ternary alloy crystals with regard to their elastic, thermodynamic and piezoelectric properties** — •Oliver Ambacher
DS 6.1	Tue	9:30–10:00	A 060	**Concerted electron-nuclear motion in polaron formation and exciton transfer** — •Wolf Gero Schmidt
DS 9.1	Wed	15:15–15:45	A 053	**Sustainable synthesis of MXenes and their precursors** — •Jesus Gonzalez-Julian, Nima Amousa, Filipa Oliveira
DS 13.1	Thu	9:30–10:00	A 053	**Computational insights into the surface functionalization and defects in MXenes** — •Hannu-Pekka Komsa
DS 13.5	Thu	11:00–11:30	A 053	**MXenes as materials for carbon capture, storage, and usage technologies: Computational insights & predictions** — •Francesc Viñes
DS 16.1	Thu	15:00–15:30	A 053	**Heterogeneous catalysis with MXenes: the role of the surface passivating groups and the structural defects** — •Alexey Fedorov
DS 16.4	Thu	16:15–16:45	A 053	**Ultrafast Photoexcitations in 2D MXenes** — •Lyubov Titova
DS 21.1	Fri	9:30–10:00	A 053	**Spotlight on Crystalline Textured Anilino-Squaraine Thin Films featuring Multiple Davydov Splitting and Charge Transfer Excitons** — •Manuela Schiek

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	**Nonequilibrium dynamics in constrained quantum many-body systems** — •Johannes Feldmeier
SYSD 1.2	Mon	10:00–10:30	H 1012	**Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics** — •Lisa-Marie Kern
SYSD 1.3	Mon	10:30–11:00	H 1012	**Interactions within and between cytoskeletal filaments** — •Charlotta Lorenz
SYSD 1.4	Mon	11:00–11:30	H 1012	**Field theories in nonequilibrium statistical mechanics: from molecules to galaxies** — •Michael te Vrugt
SYSD 1.5	Mon	11:30–12:00	H 1012	**Lightwave control of electrons in graphene** — •Tobias Weitz

Invited Talks of the joint Symposium Emerging Materials for Renewable Energy Conversion (SYEM)

See SYEM for the full program of the symposium.

SYEM 1.1	Wed	9:30–10:00	H 0105	**Non-critical Materials Production for a Green Energy Transition** — •Anke Weidenkaff, Wenjie Xie, Marc Wiedenmeyer
SYEM 1.2	Wed	10:00–10:30	H 0105	**Strategies for the morphological design of photoactive oxynitride particles and electrodes for solar water-splitting.** — •Simone Pokrant

SYEM 1.3	Wed	10:30–11:00	H 0105	**Computational workflows for an accelerated design of novel materials and interfaces** — •Ivano Eligio Castelli
SYEM 1.4	Wed	11:30–11:45	H 0105	**Autonomous composition control of emerging nitride materials for solar energy conversion** — •Andriy Zakutayev
SYEM 1.5	Wed	11:45–12:00	H 0105	**Understanding and tailoring the catalytic activity of spinel and perovskite surfaces from first principles calculations** — •Rossitza Pentcheva
SYEM 1.6	Wed	12:00–12:15	H 0105	**Mastering Compositional Complexity in High Entropy Materials for Energy Applications - Towards Accelerated Materials Discovery by Integration of High-throughput Experimentation, Simulation, and Materials Informatics** — •Alfred Ludwig

Sessions

DS 1.1–1.8	Mon	9:30–11:45	A 053	**Thin Oxides and Oxide Layers (joint session DS/KFM)**
DS 2.1–2.10	Mon	9:30–12:15	A 060	**2D Materials and their Heterostructures I: hBN, WSe2, MoS2**
DS 3.1–3.9	Mon	15:00–18:00	A 053	**Layer Properties**
DS 4.1–4.5	Mon	16:00–17:15	A 060	**Layer Deposition**
DS 5.1–5.8	Tue	9:30–11:45	A 053	**2D Materials and their Heterostructures II: Graphene and Graphene Containing Heterostructures**
DS 6.1–6.10	Tue	9:30–12:45	A 060	**Thin Film Properties I**
DS 7.1–7.8	Wed	9:30–11:45	A 053	**2D Materials and their Heterostructures III**
DS 8.1–8.10	Wed	9:30–12:30	A 060	**Thin Film Properties II**
DS 9.1–9.6	Wed	15:00–17:00	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides I (joint session DS/MM/O)**
DS 10.1–10.12	Wed	15:00–18:15	A 060	**Thin Film Application**
DS 11.1–11.31	Wed	17:00–19:00	Poster B	**Poster I (joint session DS/MM/O)**
DS 12.1–12.1	Wed	17:30–18:00	A 053	**Hertha Spohner Prize Talk**
DS 13.1–13.8	Thu	9:30–12:15	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides II (joint session DS/MM/O)**
DS 14.1–14.3	Thu	9:30–10:15	A 060	**Transport Properties**
DS 15.1–15.6	Thu	10:30–12:00	A 060	**Thermoelectric and Phase Change Materials**
DS 16.1–16.7	Thu	15:00–17:30	A 053	**Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides III (joint session DS/MM/O)**
DS 17.1–17.6	Thu	15:00–16:30	A 060	**Organic Thin Films, Organic-Inorganic Interfaces**
DS 18.1–18.3	Thu	17:00–17:45	A 060	**Optical Analysis of Organic Thin Films**
DS 19	Thu	18:00–19:00	A 053	**Members' Assembly**
DS 20.1–20.36	Thu	18:00–20:30	Poster D	**Poster II**
DS 21.1–21.9	Fri	9:30–12:15	A 053	**Optical Analysis of Thin Films**

Members' Assembly of the Thin Films Division

Thursday 18:00–19:00 A 053

DS 1: Thin Oxides and Oxide Layers (joint session DS/KFM)

Time: Monday 9:30–11:45 Location: A 053

DS 1.1 Mon 9:30 A 053

Non-collinear spin texture in thin rare-earth ion doped nickel ferrite films — •Anupam K. Singh[1], Katayoon Mohseni[1], Malleshwara R. Tangi[1], Verena Ney[2], Andreas Ney[2], Arthur Ernst[2], Yicheng Guan[1], Manuel Valvidares[3], P. Gargiani[3], Ilya Kostanvoskiy[1], Holger L. Meyerheim[1], and Stuart S. P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120, Halle (Saale), Germany — [2]Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria — [3]ALBA Synchrotron, E-08290 Cerdanyola del Valle's, Barcelona, Spain

Ferrites are abundantly used as magnetic materials, but thus far, the detailed magnetic structure in ultra-thin films has escaped clear-cut characterization. The recent observation of rare-earth-induced DMI in low-dissipation insulating oxides calls for a deeper insight into their spin texture [1]. We have studied the atomic and magnetic structure of 5 to 40 nm thick Dy-doped (5%) Zn/Al-substituted nickel ferrite (Ni0.65Zn0.35Al0.8Fe1.2O4) films prepared by magnetron sputtering. Characterization by RBS, XRD, EXAFS and XMCD experiments at the Fe-K, L2,3 and the Dy-L2,3, M4,5 edges establish the formation of a tetragonally distorted spinel structure where Dy3+ ions occupy octahedral sites with a redistribution of the Fe2+ and Fe3+ cations. Temperature-dependent SQUID, XMCD and MOKE experiments indicate a spin-reorientation transition from in-plane easy axis below 200 K, thereby showing a non-monotonic behavior of the M(T) curve which is interpreted as due to the formation of a non-collinear spin structure. [1] L. Caretta, et al., Nat. Comm. 11, 1090 (2020).

DS 1.2 Mon 9:45 A 053

Defect and Strain Engineering in SrTiO3 and CaTiO3 Thin Films Epitaxially Grown by Metal Organic Vapor Phase Epitaxy (MOVPE) — •Mohamed Abdeldayem, Changming Liu, Izaz-Ali Shah, Andreas Fiedler, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Neuromorphic devices attempt to imitate the human brain, and replace the conventional computer design to meet the demands of energy efficiency, and learning capacity. Memristive devices are a leading candidate to provide the physical properties needed for an artificial neural network. Here, we report a model in SrTiO3 and CaTiO3 thin films where resistive switching mechanism is based on polar nano-regions created by the formation of Ti anti-site defects in A-cation deficient growth regime. SrTiO3 and CaTiO3 thin films were grown epitaxially by metal-organic vapor phase epitaxy in which growth takes place near thermodynamic equilibrium and high oxygen partial pressure. This provides well-ordered epitaxial films with low defect density and negligible amount of oxygen vacancies. Moreover, chemical elements can be independently controlled by controlling the precursor fluxes in the gas phase, which enables the growth of stoichiometric and intentionally off-stoichiometric films. HRXRD, and AFM were used to verify epitaxial growth of high structural quality films with smooth surfaces. STEM-HAADF was utilized for detailed microscopic structural investigation, and showed the high homogeneity of stoichiometric films opposite to the intentionally defect ones with cloudy contrast and defect clustering.

DS 1.3 Mon 10:00 A 053

Electronic Reconstruction and Anomalous Hall Effect in the LaAlO3/SrRuO3 Heterostructure — •Merit Spring[1,2,3], Ji Soo Lim[1,2], Martin Kamp[1,4], Matthias Schmitt[1,2,3], Deepnarayan Biswas[3], Louis Veyrat[5], Pavel Potapov[5], Axel Lubk[5], Bernd Büchner[5], Tien-Lin Lee[3], Michael Sing[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Würzburg, GER — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Diamond Lightsource Ltd., Didcot, UK — [4]Wilhelm Conrad Röntgen-Center for Complex Material Systems, Universität Würzburg, GER — [5]Leibnitz Institute for Solid State and Materials Research, Dresden, GER

For the LaAlO3/SrRuO3 (LAO/SRO) system a similar electronic reconstruction to that of LaAlO3/SrTiO3 (LAO/STO) is expected, and charge is thought to be accumulated at the very interface giving rise to strong inversion-symmetry breaking and causing a topological transition of the electronic bands [1]. We show that the LAO capping drives the SRO, which turns insulating below 8 unit cells (uc) without capping, (deeper) into the metallic regime. Furthermore, we find not only signatures of an anomalous Hall effect (AHE) in 4 uc SRO films capped with LAO, but also an inversion of the sign of the AHE, when the 4uc SRO is replaced by metallic 10 uc of SRO indicating the topological phase transition. Moreover, we correlate these findings with hard and soft x-ray photoemission spectroscopy data, that show changes in the ruthenium electronic states, and discuss these changes in terms of correlated electrons. [1] Thiel, T. C. et al., Phys. Rev. Lett. 127, 127202 (2021)

DS 1.4 Mon 10:15 A 053

Exploration of zirconium doping in pulsed laser deposited α-Ga_2O_3 for devices — •Sofie Vogt[1], Thorsten Schultz[2,3], Clemens Petersen[1], Holger von Wenckstern[1], Norbert Koch[2,3], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut, Leipzig — [2]Humboldt Universität zu Berlin, Institut für Physik, Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Solar Energy, Berlin

Gallium oxide, known for its ultrawide bandgap, crystallizes in different polymorphs, of which the β-phase is the thermodynamically most stable and most investigated one. However, the metastable corundum structured α-phase exhibits a wider bandgap and therefore a potentially higher electrical breakdown field compared to β-Ga_2O_3[1]. Doping of α-Ga_2O_3 with tin, silicon and germanium has been demonstrated[2,3]. We present α-Ga_2O_3 thin films grown by pulsed laser deposition in a two-step process. Undoped α-Ga_2O_3 grown at high temperature is used as buffer layer. The zirconium doped α-Ga_2O_3 is deposited atop the buffer layer at a temperature $< 600°C$, to ensure the deposition of conductive thin films. The structural and electrical properties of Zr doped thin films are compared to Sn, Si and Ge doped thin films with regards to the crystal quality, conductivity, free carrier concentration and electron mobility. First Schottky barrier diodes based on the α-Ga_2O_3:Zr thin films are presented.

[1] Higashiwaki *et al.*, Appl. Phys. Lett., **100**, 013504 (2012)
[2] Akaiwa *et al.*, phys. status solidi (a), **217**, 3, 1900632 (2020)
[3] Vogt *et al.*, phys. status solidi (a), **220**, 3, 2200721 (2023)

15 min. break

DS 1.5 Mon 10:45 A 053

Epitaxy and transfer of freestanding $SrTiO_3$ membranes — •Jeremy Maltitz, Weaam Ayad, Jens Martin, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

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 perovskite thin films have been achieved by introducing a perovskite-like, water-soluble sacrificial layer (Sr3Al2O6) between substrate and functional film. In combination with layer transfer, this provides a playground for fundamental investigations and technological applications of complex oxides beyond the limitations of classical heteroepitaxy. Requirements are the preparation of epitaxial oxide films with high structural quality of both sacrificial layer and functional oxide film and the controlled detachment from the growth substrate and transfer on another substrate. In this contribution, we will show the influence of the PLD parameters, film thicknesses and composition of the oxide films on the release process and crack formation in freestanding SrTiO3 thin films by using the solid-solution family of (Ba,Ca,Sr)3Al2O6 as sacrificial layer. While cracking of the SrTiO3 films during etching of the sacrificial layer can be largely avoided by the growth of an almost strain-free heterostructure, the transfer process remains challenging. One approach is the use of sub-mm small polymer stamps to transfer deliberately smaller pieces of the functional oxide film on the target substrate.

DS 1.6 Mon 11:00 A 053

Investigation of electrical properties of metal oxide semiconductors thinfilms — •Pinar Oruc[1], Ali Orkun Cagirtekin[1], Sukru Cavdar[1], Nihat Tugluoglu[2], and Haluk Koralay[1] — [1]Gazi University, Faculty of Science Department of Physics, Ankara Turkiye. — [2]Giresun University, Faculty of Engineering, Department of Energy Engineering, Giresun, Turkiye.

Metal oxide semiconductor materials such as TiO2, ZnO, V2O5, and

MoO3 have very large technological area because of their useful properties [1]. Generally, these materials are interesting by scientific community because they have wide forbidden energy band gap, good electrical, and optical properties [2]. With the development of technology, the development of higher performance and cost-effective devices has become more important. For these reasons, the importance of these semiconductor metal oxide structures has gradually increased. In this study, electrical characterization of multilayer semiconductors device was investigated. Different metal oxide thin film layers were grown on the fluorine doped tin oxide (FTO) substrate by using different methods. It has been observed that both thin films obtained with different techniques have a homogeneous surface. Electrical measurements of the device were taken at different temperatures, widely frequency regions. As a result of electrical measurements, the device showed good diode behavior also electrical behavior of the fabricated device showed better electrical properties as the increasing temperature. According to the results, the fabricated device can be used many electronic areas.

DS 1.7 Mon 11:15 A 053

Engineering electrochemical conversion in La_2NiMnO_6 using magnetic ground states — •Pia Henning and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

For a more sustainable future, the identification of new electrocatalyst materials for the oxygen evolution reaction (OER) plays an important role. In the course of this, the oxide double perovskite La_2NiMnO_6 exhibits a promising role [1]. Especially interesting for this material is the interplay between magnetic ground state and OER activity. The catalytic activity of La_2NiMnO_6 powder samples is enhanced when a vibronic superexchange interaction is present, dominating over static exchange interactions [1]. However, the magnetic structure is closely linked to the oxygen content in the sample and a low Curie temperature can also be originating from oxygen vacancies in the lattice [2]. To resolve this, we prepared La_2NiMnO_6 thin films with our hybrid PLD set-up, combining standard PLD with MBE techniques. The samples were carefully modified by controlling the oxygen content. These modifications of the B-site electronic configuration were then related to the OER activities of the samples, using the magnetic properties as descriptor.

[1] Y. Tong, J. Wu, P. Chen, H. Liu, W. Chu, C. Wu, Y. Xie, Journal of the American Chemical Society 2018, 140(36), 11165.

[2] J. P. Palakkal, T. Schneider, L. Alff, AIP Advances 2022, 12(3), 035116.

DS 1.8 Mon 11:30 A 053

Ferroelectric polarization rotation through He irradiation induced uniaxial strain — •Andreas Herklotz[1], Robert Roth[1], Kathrin Dörr[1], Alessandro Mazza[2], and Thomas Zac Ward[3] — [1]1) Institute for Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany — [2]2) Los Alamos National Laboratory, Los Alamos, USA — [3]3) Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA

The physical properties of ferroic thin films are typically dominated by their domain configurations and their responses to external fields. A central prerequisite to domain engineering and harnessing functionalities of ferroelectric thin films is thus the control of the polarization orientation. Historically, the symmetry of ferroelectric films has been mainly tailored by heteroepitaxial in-plane strain or a variation of growth conditions inducing defects.

Here, we deploy low-energy He implantation as an alternative approach. Ion implantation induces uniaxial out-of-plane strain, while the in-plane strain remains fixed due to epitaxial constraint. We show that this kind of uniaxial strain engineering effectively leads to polarization rotation from in-plane towards out-of-plane as the uniaxial strain is increasing. We find that this polarization rotation can be achieved via two different mechanisms: (i) via a sequence of phase transitions related to changes of crystal symmetries and (ii) via a continuous shift of the ferroelectric domain ratio towards out-of-plane oriented domains.

DS 2: 2D Materials and their Heterostructures I: hBN, WSe2, MoS2

Time: Monday 9:30–12:15 Location: A 060

DS 2.1 Mon 9:30 A 060

Strain activation of negatively charged boron vacancies in hexagonal boron nitride — •Xuankai Zhou[1], Jianpei Geng[2], Ruoming Peng[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, University of Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart, Germany — [2]School of Physics, Hefei University of Technology, Hefei 230009, China

Spin defects in 2-dimensional materials have been extensively investigated since they offer a new playground for novel quantum phenomena, with improved scalability in device fabrication and the ability to study field and strain modulation. Negatively charged boron vacancy in hexagonal boron nitride (hBN) has been identified as an optically activated spin defect, hosting spin-1 ground states for quantum sensing. However, the emitted light from implanted boron vacancies tends to be dim, limiting their sensitivity. In this study, we made an important observation that the brightness of V_B^- is substantially enhanced when these vacancies are situated within the wrinkles and dislocations of hBN. Specifically, for hBN with a thickness of approximately 10 nm, we observed a remarkable increase of more than an order of magnitude in emission brightness, combined with an improved Optically Detected Magnetic Resonance (ODMR) contrast. Our findings shed light on the modulation of excited-state symmetry and the dynamics of underlying intermediate states in hBN induced by local strain and structure dislocation.

DS 2.2 Mon 9:45 A 060

Defect creation in hexagonal boron nitride by plasma treatment — •David Plitt, Felix Schaumburg, Timo Wagner, Martin Geller, Günther Prinz, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Hexagonal boron nitride (hBN) gained great attention after it was experimentally proven that their color centers exhibit single photon emission properties[1]. Simulations suggest that the emission wavelength of these color centers range from IR to UV[2], which was confirmed in experiments too[3]. Our measurements show that it is possible to create different color centers in the hBN structure using plasma treatment. This was achieved using different gases (argon, nitrogen and oxygen) and plasma parameters, including pressure, excitation power and distance to the plasma. The resulting color centers were then analyzed with photoluminescence measurements. Different excitation laser wavelengths were used and the measurements were conducted at room temperature as well as at low tempeatures. The produced defects cover the spectral range between 400 nm and 750 nm. A portion of the color centers exhibit time dependent optical properties like blinking and a shift in the emission wavelength.

[1] Zai-Quan Xu et. al., Nanoscale, 2018, 10, 7957 [2] Mehdi Abdi et. al., ACS Photonics 2018, 5, 1967-1976 [3] Suk Hyun Kim et. al., Nanomaterials 2023, 13, 2344

DS 2.3 Mon 10:00 A 060

Exciton-exciton interactions in heterobilayers of transition-metal dichalcogenides — •Edith Wietek[1], Alexander Steinhoff[2], Matthias Florian[3], Tommy Schulz[2], Takashi Taniguchi[4], Kenji Watanabe[4], Shen Zhao[5], Alexander Högele[5], Frank Jahnke[2], and Alexey Chernikov[1] — [1]Technische Universität Dresden, Deutschland — [2]Universität Bremen, Deutschland — [3]University of Michigan, USA — [4]NIMS, Ibaraki, Japan — [5]LMU München, Deutschland

Vertically stacked heterostructures of transition metal dichalcogenides (TMDCs) offer a versatile platform to study electronic and excitonic many-body effects. In particular, interactions between interlayer excitons are key to understand both non-linear optical and transport phenomena in these systems. Here, we address this topic in a joint experiment-theory study by considering spectrally narrow interlayer excitons in the moiré free limit of atomically reconstructed, hBN-encapsulated MoSe2/WSe2 heterobilayers. While classical dipolar repulsion is broadly assumed to determine exciton-exciton scattering, we demonstrate a major role of additional many-body effects includ-

ing exchange interaction and dynamic screening. Identified by theory, these contribution compensate dipolar term, accounting for the observed spectral shifts of the interlayer excitons of only a few meV even for high injection densities close to the Mott transition threshold. Our findings challenge the traditional picture of the dipolar repulsion in van der Waals heterostructures, highlighting the major role of exchange and screening for the exciton-exciton interactions.

DS 2.4 Mon 10:15 A 060

Dielectric Function and exciton dynamics of 2-dimensional MoS_2 — •Lucas Krätschmer[1], Younes Slimi[1], Lukas Trefflich[2], Theo Pflug[3], Markus Olbrich[3], Noah Stiehm[1], Bernd Hähnlein[1], Sebastian Thiele[1], Chris Sturm[2], Alexander Horn[3], Marius Grundmann[2], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Technische Universität Ilmenau, Ilmenau, Deutschland — [2]Universität Leipzig, Leipzig, Deutschland — [3]Hochschule Mittweida, Mittweida, Deutschland

2-dimensional MoS_2 belongs to the Transition Metal Dichalcogenide (TMD) family with a band gap of 1.7 eV, and thus has unique properties for optoelectronic applications. We present the dielectric function of a homogeneous MoS_2 film deposited on a sapphire substrate with a size of 1cm x 1cm in the spectral range of 0.5 to 6.5 eV. The sample was purchased commercially from the company Ossila B.V.. The static optical properties of the sample were determined by spectroscopic ellipsometry (SE), spatially integrated as well as spatially resolved to survey the local optical properties of the sample. We found that the integrated as well as the local optical response is quite similar, showing high homogenity of the film. We found further indications for grain boundaries (grain size approx. 1 μm) from the Ψ- and Δ-Maps. Based on these results, time-resolved imaging ellipsometry measurements are planned to investigate the dynamics of the exciton propagation.

DS 2.5 Mon 10:30 A 060

Photo-induced charge and spin transfer in the heterostructure $CrSBr/MoSe_2$ — •Andreas Beer[1], C. Serati de Brito[1,2], K. Zollner[1], P. E. Feria Junior[1], J. Fabian[1], H. S. J. van der Zant[3], Y. Galvao Gobato[2], and C. Schüller[1] — [1]University of Regensburg — [2]Universida de Federal de Sao Carlos — [3]Delft University of Technology

Van der Waals (vdW) heterostructures composed of two-dimensional (2D) transition metal dichalcogenides (TMDC) and vdW magnetic materials offer an intriguing platform to functionalize valley and excitonic properties in non-magnetic TMDCs. Here, we report a two color pump probe investigation of monolayer (ML) $MoSe_2$ on the layered A-type antiferromagnetic (AFM) semiconductor CrSBr. The material combination is predicted to feature a type III band alignment (broken bandgap), which leads to an p-doping in $MoSe_2$. This can already be suspected by photoluminescence, white light mapping and magneto-PL measurements, but can ultimately be shown by a pump probe technique. An ultrafast pump pulse creates free electrons in CrSBr. They can tunnel to $MoSe_2$ and reduce the background doping. The reduction can then be detected by an enhancement (reduction) in reflectivity of the $MoSe_2$ exciton (Trion). Remarkably by pumping the heterostructure with circular polarized light we can observe a long-lasting Kerr effect in the heterostructure. We explain our results by an out of plane spin component in the first layer of CrSBr.

15 min. break

DS 2.6 Mon 11:00 A 060

Photo-electrochemical thinning of transition metal dichalcogenides — •Simon Wörle[1], Jeremy Robinson[2], Franz Gröbmeyer[3], Emiliano Cortes[3], and Ian Sharp[1] — [1]Technical University of Munich — [2]Naval Research Laboratory, Washington, D.C — [3]Ludwig-Maximilians-Universität München

Two-dimensional transition metal dichalcogenides have attracted considerable attention due to their unique optoelectronic, mechanical and catalytic capabilities. For the application of 2D materials in semiconductor devices, the precise control of their properties is crucial, with the layer number being the most fundamental. Here, we demonstrate a top-down approach in aqueous solutions and under illumination to thin MoS_2, WS_2, $MoSe_2$ and WSe_2 layers of various thicknesses down to, in some cases, a self-limiting number of layers. The removal of the upper layers is initiated by laser illumination with wavelengths of 532nm and 785nm. In contrast to laser degradation in air, where the TMD layers heat and sublimate, the thinning procedure in water is electrochemically driven. Photo-excited holes oxidize the surface layers in a self-limiting mechanism. An additional external voltage applied against a defined reference potential allows this thinning process to be further enhanced or prevented. For potentials larger than 0.8V vs Ag/AgCl, the thinning of MoS_2 occurs even under white light microscope illumination. The oxidation, starting at the edges or defects and spreading through the whole TMD flakes, can be in-situ monitored. The presented results show an overview of photo-electrochemical thinning of different TMDs under various bias and excitation conditions.

DS 2.7 Mon 11:15 A 060

DFT-assisted Investigation of Defects in 2D WSe2 by High-Resolution STEM and Differential Phase Contrast Imaging — •Maja Groll, Julius Bürger, Ioannis Caltzidis, Klaus D. Jöns, Wolf Gero Schmidt, Uwe Gerstmann, and Jörg K. N. Lindner — Department of Physics, Paderborn University, Germany

2D transition metal dichalcogenides and defects therein are currently the subject of intensive research due to their extraordinary optoelectronic properties. In particular, defects in monolayers, typically of vacancy type, are attracting much attention. Most spectroscopic investigations of material properties caused by defects are limited by the spatial resolution far above the atomic level. However, knowledge of the atomic structure is crucial for a detailed understanding of these properties. Modern scanning transmission electron microscopy (STEM) in combination with differential phase contrast imaging (DPC) allows for a structural analysis combined with the investigation of the electric field distribution at sub-atomic resolution. This enables the identification of defects and the resulting change in the field distribution. However, interpretation of STEM data is demanding because single substitutional atoms, such as oxygen, are difficult to detect and can nevertheless influence the physical and chemical properties. Here, vacancies in mechanically exfoliated 2D WSe2 flakes are analysed with focus on possible substitutional atoms. Conventional STEM at an acceleration voltage of 80keV in combination with STEM-DPC and density functional theory (DFT) calculations are used to characterize point defects and investigate their charge density distribution.

DS 2.8 Mon 11:30 A 060

Light-Matter coupling in Van der Waals heterostructures — •Bharti Parashar, Mathias Federolf, Atanu Patra, Vishakha Kaushik, and Sven Höfling — Technische Physik, University of Würzburg, Am Hubland 97074 Würzburg Germany

Transition metal dichalcogenides (TMDCs) heterostructures (HSs) offer a dynamic platform where artificially stacked monolayers of different TMDCs materials may reveal intriguing quantum behaviors. The alignment or twist between these monolayers generates a periodic moiré pattern, endowing the presence of the quasi-particle intralayer exciton, within the same material and an interlayer exciton characterized by charge carriers originating from different monolayers. Moiré superlattices in two-dimensional (2D) HSs induce quantum phenomena by fundamentally altering the electronic hybridizations by controlling the twist angle between atomically thin layers. This paradigm shift provides a unique avenue for precisely tailoring interactions between quantum particles and their coupling to electromagnetic fields. Moreover, beyond their discernible effects on single-particle states, strong moiré superlattices manifest excited states, such as the formation of moiré minibands of excitons [1]. In this study, we comprehensively explore the optoelectronic characteristics of twisted WSe2/WS2 van der Waals HSs. The insights obtained contribute to establishing a foundational understanding essential for realizing many-body states in moiré superlattices, such as exciton condensates, and bosonic insulating states via electric field manipulation.

Ref: [1] Jin, Chenhao, et al. Nature 567.7746 (2019): 76-80

DS 2.9 Mon 11:45 A 060

Large-area epitaxial growth and investigation of $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Michael Hanke[1], Jens Herfort[1], Achim Trampert[1], Roman Engel-Herbert[1], Chen Chen[2], Joan Redwing[2], Manfred Ramsteiner[1], and J Marcelo Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, Pennsylvania, United States

Van der Waals heterostructures (vdWH) consisting of two-dimensional ferromagnets and transition metal dichalcogenides have attracted great interests due to their promising (opto)spintronic applications.

The $Fe_{5-x}GeTe_2$ (FGT, with x $\sim$ 0.2) is considered as one of the most promising materials due to its high-temperature ferromagnetic order and robust perpendicular magnetic anisotropy (PMA). We report on the large-area MBE growth of FGT on CVD-grown $WSe_2/Al_2O_3(0001)$. The structural characterizations reveal the high-quality formation of FGT/WSe_2 vdWH. The anomalous Hall effect (AHE) exhibits a clear hysteresis loop below 250 K providing evidence for PMA. The S-shaped AHE at higher temperatures indicates a magnetic order up to 360 K. Further magnetotransport anomaly can be explained by the formation of skyrmions accompanied by a topological Hall effect and a non-colinear magnetic order contribution to the magnetoresistance. Our results demonstrate the extraordinary potential of high-quality FGT/WSe_2 vdWH for tailoring proximity-induced phenomena that can be exploited for (opto)spintronic applications.

DS 2.10 Mon 12:00 A 060

multi-strategy coordination enables WSe2 to achieve high-performance real-world detection of NO2 — •Yu Duan[1,2], Sam Zhang[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Advanced Thin Films and Devices, School of Materials and Energy, Southwest University, Chongqing, 400715, China

In recent years, WSe2 has become an ideal material for room-temperature NO2 gas sensing, but its low response and long response time limit its application. In this study, we combined multiple strategies of constructing a three-dimensional structure, introducing Se vacancies, Au nanoparticle sensitization, and 1T/2H-phase modulation. The synergistic effect was utilized to effectively enhance the gas adsorption, charge transfer degree, and carrier transport capacity of WSe2 and achieve high-performance NO2 detection. The prepared V-WAAP achieved high response (78.32%) with a short response time (33 s), and outstanding stability and selectivity for low concentration (1 ppm) NO2. The intrinsic factors of sensing performance improvement were comprehensively analyzed by combining the results of compositional and structural characterization. In addition, we verified its potential for practical applications by assembling a V-WAAP-based NO2 gas sensing equipment.

DS 3: Layer Properties

Time: Monday 15:00–18:00 Location: A 053

Invited Talk DS 3.1 Mon 15:00 A 053

Advances in AlN-based ternary alloy crystals with regard to their elastic, thermodynamic and piezoelectric properties — •Oliver Ambacher — Institute for Sustainable System Engineering, University Freiburg

The piezoelectric coefficient e33 from wurtzite AlN (wz-AlN), which is particularly interesting for high-frequency acoustic wave filters, can be increased up to 150% by alloying AlN with ScN or YbN. In addition, wz-ScAlN and wz-YbAlN layers show ferroelectric properties and large remanent polarizations up to very high temperatures. The ferroelectric effect enriches the dimension of polarization engineering in group-III-nitride based heterostructures and provides opportunities for the integration of novel functionalities into electronic and piezo acoustic devices. For this reason the piezoelectric, spontaneous, and ferroelectric polarization as wll as the structural, elastic, and thermodynamic properties of hexagonal GaN, ScN, YbN and AlN crystals as well as their ternary alloy will be presented.

DS 3.2 Mon 15:30 A 053

Eliminating oxygen in-diffusion for stabilization of electrical properties in CuI thin films — •Christiane Dethloff, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institut, Universität Leipzig, Deutschland

The p-type semiconductor CuI is of great potential for transparent opto-electronics due to an intrinsic charge carrier density of up to 10^{20} cm^{-3} combined with a direct band gap of 2.95 eV at room temperature and high transparency in the visible range [1,2]. The p-type behavior is attributed to Cu vacancies, but recently also to oxygen, which acts as a shallow acceptor. It was demonstrated that in particular ex-situ oxygen diffusion causes an increase of hole density and electrical conductivity, often resulting in degenerate thin films [2].
To access the full potential of CuI and its alloys for semiconductor thin film applications, it is crucial to prevent in-diffusion of oxygen. Although amorphous Al_2O_3 capping layers atop CuI thin films have already been shown to prolongate deterioration of the electrical properties, the influence of a full encapsulation has not yet been investigated. Therefore, we present completely *in-situ* encapsulated CuI thin films deposited by magnetron co-sputtering from a Cu target in a reactive iodine and argon atmosphere. We compare the efficiency of Al_2O_3 and SiN_x cappings that encapsulate the surface and the entire layers, respectively. For that, long-term resistivity and Hall effect measurements are performed over several days.
[1] Yang *et al.* Nat Commun **8**, 16076 (2017).
[2] Storm *et al.* APL Mater. **9** (5): 051101 (2021).

DS 3.3 Mon 15:45 A 053

Understanding of the Cu nanofilament behavior of Cu/HfO2/Pt with QPC model — •Taewook Kim[1], Enrique Miranda[2], Eszter Piros[1], Philipp Schreyer[1], and Lambert Alff[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Universitat Autonoma de Barcelona, Barcelona, Spain

This study delves into the behavior of the Cu conducting filament in a Cu/HfO2/Pt MIM (Metal-Insulator-Metal) structure, specifically examining resistive switching mechanisms in filamentary-type memory. Utilizing the Quantum Point Contact (QPC) model, we analyze the Cu conducting filament's response to variations in oxide layer thickness. The investigation reveals distinct conducting filament behaviors associated with different oxide layer thicknesses. Thinner oxide layers result in a smaller energy barrier between ruptured filaments, while thicker oxide layers exhibit a higher energy barrier. Furthermore, thicker oxide layers show an increased ratio of broken parts, suggesting significant rupturing of the Cu conducting filament in thicker oxide layer sample. The study extends to examining the possible conduction mechanism post-rupturing, as evidenced by a comparison of the I-V curve between set and reset states. This research provides crucial insights into the intricacies of resistive switching in MIM structures, with potential applications in memory devices and contributions to the advancement of nanoscale electronics.

15 min. break

DS 3.4 Mon 16:15 A 053

Are Xenes excitonic insulators? — •Olivia Pulci[1], Paola Gori[2], Davide Grassano[3], Marco D'Alessandro[4], and Friedhelm Bechstedt[5] — [1]Department of Physics, and INFN, University of Rome Tor Vergata, Italy — [2]Department of Industrial, Electronic and Mechanical Engineering, Roma Tre University, Italy — [3]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, Switzerland — [4]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [5]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany

Using a variational approach, the binding energies Eb of the lowest bound excitons in Xenes under varying electric field are investigated. The internal exciton motion is described both by Dirac electron dispersion and in effective-mass approximation, while the screened electron-hole attraction is modeled by a Rytova-Keldysh potential with a 2D electronic polarizability α2D. The relation between Eb and the spin-orbit gap Eg is ruled by the screening. The values of Eg and α2D are strongly modified by a vertical external electric bias U, which defines a transition from the topological into a trivial insulator at U = Eg /2, with the exception of plumbene. The existence of an excitonic insulator phase with Eb>Eg sensitively depends on the chosen α2D. Many-Body perturbation theory, applied to stanene, confirm the absence of an excitonic insulator phase, thus validating our results obtained by ab initio modeling of α2D.

DS 3.5 Mon 16:30 A 053

Electrical characterization of the pseudo-binary line In_3SbTe_2-SnTe — •Christian Stenz, Thomas Schmidt, Michael Dappen, and Matthias Wuttig — I. Institute of Physics (IA)

RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen

Materials can be categorized by examining their properties, including band gap, effective coordination number, electrical and optical conductivity, Born effective charge, and more. Based on such properties and quantum chemical bond identifiers a classification into metallic, covalent, ionic, and metavalent bonding (MVB) appears appropriate. MVB is defined by a competition between electron localization and delocalization resulting in a unique property portfolio. SnTe and In_3SbTe_2 are identified to be metavalent and metallic, respectively. However, both occur in a rocksalt-like structure with similar lattice constants allowing for isostructural alloying. Investigating the property portfolio of the pseudo-binary line yields insights about the pronounced changes in properties by crossing the tipping point towards complete electron delocalization and closing the band gap. In this study several alloys on the pseudo-binary line In_3SbTe_2-SnTe are produced by sputter deposition. Properties like crystallization temperature T_x, electrical conductivity and superconducting transition temperature T_c are investigated. Upon the transition from MVB to metallic bonding a change in charge carrier type as well as a remarkable increase of T_c by 85 % and 1200 % compared to the pure compounds In_3SbTe_2 and SnTe, respectively, has been found.

DS 3.6 Mon 16:45 A 053

Mesoscale modeling of deformations and defects in crystalline sheets — •Lucas Benoit–Maréchal[1], Ingo Nitschke[1], Axel Voigt[1,2], and Marco Salvalaglio[1,2] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

We present a self-consistent mesoscale description of deformations and defects in thin, flexible sheets with crystalline order using a coarse-grained Phase-Field Crystal (PFC) model which aims at bridging atomistic and continuum approaches.

The PFC model describes crystals at diffusive timescales through a continuous periodic field representing the atomic number density. In its amplitude expansion (APFC), a coarse-grained description featuring slowly varying fields retaining lattice deformation, elasticity, and dislocations is achieved. We introduce the surface APFC (sAPFC) model in a convenient height formulation encoding normal deformation.

This framework is proven consistent with classical aspects of strain-induced buckling, defect nucleation on deformed surfaces, and out-of-plane relaxation near dislocations obtained from atomistic and continuum descriptions. By considering the mutual interaction of elastic/plastic relaxation and variations in the height profile as accessible within the sAPFC model, we outline the complexity of the resulting phenomenology.

15 min. break

DS 3.7 Mon 17:15 A 053

Multiscale Simulation Framework for Functional Polymers — •Steffen Kampmann[1], Alexander Croy[2], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden, Dresden, Germany — [2]Chair of Theoretical Chemistry, Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Functional mechanically resilient polymer films, such as films of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), play an important role for strain gauges or organic light-emitting diode (OLED) displays [1-2]. The modeling and simulation workflow presented here enables the generation of disordered polymers and the linking of the mechanical and electronic properties from the atomistic to the microscopic size scale. Here, the focus is on the relationship between deformation and conductivity behavior. To calculate the multi-scale material behavior, we use density functional tight binding (DFTB) calculations, molecular dynamics simulations, and the finite element method. The in-situ processing, evaluation as well as the exchange of the generated data across simulation methods is performed using our Python framework. The multi-scale computational workflow indicated here represents a computationally efficient assessment of material properties at different scales. [1] R. Luo, et al., Progress in Organic Coatings, (2022) [2] M. Cinquino et al., Journal of Science: Advanced Materials and Devices, (2022)

DS 3.8 Mon 17:30 A 053

Controllable phase transition of two-dimensional ferromagnetic chromium telluride thin films grown by molecular beam epitaxy — •Haili Huang — Shanghai Jiao Tong University

Two-dimensional (2D) Cr(1+δ)Te2 materials exhibit strong magnetic ordering and high Curie temperatures, making them attractive for various applications. However, it is crucial to achieve controllable synthesis for their successful integration into device technologies. In this study, we present the synthesis of phase-controllable 2D Cr(1+δ)Te2 films on the Si (111) substrate via molecular beam epitaxy. The composition and phase transition of the as-grown Cr(1+δ)Te2 films are characterized by using in-situ reflection high-energy electron diffraction, scanning tunneling microscopy, ex-situ X-ray photoelectron spectroscopy, X-ray diffraction, and theoretical calculations. By carefully adjusting the film thickness, we achieve precise control over the phase and growth mode of Cr(1+δ)Te2. These changes are attributed to interfacial effects and the phase stability of Cr(1+δ)Te2 compounds. The magnetic measurements reveal that the 30-nm Cr2Te3 film exhibits ferromagnetic behavior with a Curie temperature of about 180 K. Our work offers a robust method for the controllable growth of high-quality 2D Cr(1+δ)Te2 films on Si substrates, providing an ideal platform for investigating their intrinsic properties and advancing the development of 2D magnet-based spintronics devices.

DS 3.9 Mon 17:45 A 053

Combinatorial study of BaCu2Se2 thin films for photovoltaics — •Marin Rusu[1], José A. Márquez[1], Hannes Hempel[1], Leo Choubrac[1], Galina Gurieva[1], Rene Schwiddessen[1], Pablo Reyes-Figueroa[1], Robert Wenisch[1], Markus Schleuning[1], Christian A. Kaufmann[1], Iver Lauermann[1], Susan Schorr[1,2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

BaCu2Se2 thin films with earth-abundant elements are investigated for application in photovoltaics. We apply the combinatorial approach for the study of BaCu2Se2 thin films with a lateral gradient in the [Cu]/[Ba] atomic ratio, which were synthesized on areas as large as 5x5 cm2 by selenization of Cu-BaO precursors from pulsed laser deposition. Close to the the 1:2:2 stoichiometric point, the optical measurements revealed a direct band gap with an energy of 1.89 eV in perfect agreement with the observed bright photoluminescence centered at 1.9 eV. An absorption coefficient of 1.5 x 105 cm-1 was determined and a theoretical open-circuit voltage of 1.3 eV was calculated. By using optical-pump terahertz-probe spectroscopy mapping, as well as a combined Kelvin probe with a photoelectron yield spectroscopy method, we find that the equilibrium charge carrier concentration can be tuned over five orders of magnitude. Surface photovoltage measurements revealed a p-type conductivity of the films. The charge carrier mobility reaches a maximum value of ~60 cm2 V-1s-1. Thus, BaCu2Se2 thin films are very attractive for application in tandem photovoltaics.

DS 4: Layer Deposition

Time: Monday 16:00–17:15 Location: A 060

DS 4.1 Mon 16:00 A 060

Real-Time Investigations during Sputter Deposition on Polymer Thin Films. — •Matthias Schwartzkopf — DESY, Photon Science, Notkestr. 85, 22607 Hamburg, Germany

The reproducible low-cost fabrication of functional polymer-metal-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed time-resolved surface sensitive X-ray scattering during sputter deposition of gold on thin polystyrene films and silicon substrates [1,2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of atomic deposition rate on the growth regimes with their specific thresholds even at high deposition rates [3,4]. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013); [3] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017), [4] Schwartzkopf et al.,Nanoscale Horiz. 6, 132 (2021).

DS 4.2 Mon 16:15 A 060

Fast and efficient simulation of the FEBID process — •Alexander Kuprava and Michael Huth — Goethe University, Frankfurt, Germany

Over the last decade focused electron beam induced deposition or FEBID has been shown to be a promising technique for next generation nanofabrication. Unlike conventional lithography techniques, FEBID enables true free-form fabrication of 2D and 3D structures and opens a path for the development of novel nanomaterials. However, the shape-true transfer from a 3D CAD model to a deposit represents a serious challenge to a more widespread practical usage of the method. Different simulation approaches, e.g., and slicers or pattern optimizers have been reported, e.g., addressing various aspects of the shape-true transfer. Our effective hybrid Monte Carlo-continuum simulation of the FEBID process allows prediction of the resulting shape with the consideration of beam heating effects of the structure.

The simulation represents a material deposition model based on the dissociation of adsorbed precursor molecules by the electron beam. The deposition process is based on a reaction-diffusion continuum model describing the influence of precursor adsorption, desorption, diffusion and dissociation on the surface precursor coverage and consequently on the growth rate.

Owing to the reasonable execution speed on a regular desktop, the simulation can assist the laborious work of pattern file and parameter optimization during the fabrication of complex 3D structures.

DS 4.3 Mon 16:30 A 060

GaS - a Two-Dimensional UV emitting material: Challenges of MOCVD Synthesis — •Robin Günkel[1], Stefan Renato Kachel[1,2], Leonard Neuhaus[2], Lukas Erlemeier[2], Tigmanshu Sundrial[1], Johannes Glowatzki[1], Jürgen Belz[1], Carsten von Hänisch[2], J. Michael Gottfried[2], and Kerstin Volz[1] — [1]Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Germany — [2]Material Sciences Center and Department of Chemistry, Philipps-Universität Marburg, Germany

Gallium sulfide (GaS), a 2D semiconductor similar to Transition Metal Dichalcogenides (TMD), has a band gap in the UV wavelength range, making it a candidate for UV LED applications. The goal of this study is to synthesize a 2D GaS crystal directly on a substrate, rather than producing it by mechanical exfoliation. Metal-Organic Chemical Vapor Deposition (MOCVD) enables the controlled growth of atomically thin films. This type of synthesis is scalable, with process adaptations limited primarily by substrate size and reactor dimensions. We use established MOCVD precursors such as di-tert-butyl sulfide (DTBS) and tri-tert-butyl gallium (TTBGa). First growth experiments show excess metallic Ga remaining on the surface of the 2D layered GaS. When we try to compensate for the excess Ga by increasing the supply of sulfur, growth is inhibited. To overcome this challenge, a pulsed growth sequence rather than a continuous one is applied. Furthermore, as additional approach the surface chemistry is investigated, and the application of single source precursor is under discussion.

DS 4.4 Mon 16:45 A 060

MBE growth and characterization of α-$FeGe_2$ films on GaAs(001) — •Moritz N. L. Hansemann, Michael Hanke, Achim Trampert, and Jens Herfort — Paul Drude Institut, Berlin, Germany

Layered 2D magnets are becoming a cornerstone in the realization of spintronic devices. The layered material α-$FeGe_2$ adds to the family of magnetic materials with a ferromagnetic antiferromagnetic phase transition, predicted by density functional theory calculations (DFT).

We show the growth by molecular beam epitaxy of the novel α-Phase of $FeGe_2$ on GaAs (001) and present comprehensive structural characterization by atomic force microscopy (AFM), X-ray diffraction (XRD), and high resolution transmission electron microscopy (hR-TEM). For the growth of α-$FeGe_2$ we utilize solid phase epitaxy of amorphous Ge on Fe_3Si. Subsequent annealing reveals the layered structure of α-$FeGe_2$ in the P4mm spacegroup. Reciprocal Space Maps (RSM) and TEM images show excellent epitaxial alignment and high structural quality. We experimented with off-stoichiometric growth by buffering Ge and report the formation of Ge agglomerates (droplets) on the surface. Additionally we present initial Hall- and I-V-measurements that show possible semimetallic behavior.

DS 4.5 Mon 17:00 A 060

Energetische Anpassung von Magnetron-Sputter-Abscheidungsprozessen für defektempfindliche Materialien: Transparente leitfähige Oxide und andere Halbleiter — •Klaus Ellmer — Optotransmitter-Umweltschutz-Technologie e.V., Köpenicker Str. 325, 12555 Berlin, Germany

Das Magnetronsputtern ist eine großflächige, plasmaunterstützte Abscheidungsmethode für viele industrielle Anwendungen, wie Architektur- und Glasbeschichtungen, von Spiegeln und Absorbern für Solarkonzentratoren, magnetische Schichten für Festplatten oder Hartstoffschichten. In der Dünnschicht-Photovoltaikindustrie wird Magnetronsputtern zur Abscheidung metallischer Rückkontakte (Ag, Mo) und transparenter, leitfähiger Fensterschichten (ITO, ZnO) oder für metallische Filme eingesetzt. Für die aktiven Halbleiter (Absorber) in Solarzellen wird es jedoch noch nicht im technischen Maßstab angewendet. Es werden Hindernisse aufgezeigt, die den Einsatz des Magnetronsputterns für aktive Halbleiterschichten verzögert haben. Die Energien der Spezies (gesputterte Atome, positive und negative Ionen, energiereiche Neutrale) werden diskutiert und ihr Einfluss auf das Filmwachstum. Aufgrund der geringen Defektbildungsenergien von Halbleitern ist die Anpassung der Entladungsbedingungen (niedrige Teilchenenergien) für die Herstellung defektarmer Halbleiterfilme mit hoher Qualität zwingend erforderlich. Die Möglichkeiten des Magnetronsputterns werden für die Abscheidung aktiver Chalkopyrit-Absorberfilme für effiziente Solarzellen (Cu(In,Ga)Se2), für Nitride für LEDs (GaInN) und für transparente leitende Oxide demonstriert.

DS 5: 2D Materials and their Heterostructures II: Graphene and Graphene Containing Heterostructures

Time: Tuesday 9:30–11:45 Location: A 053

DS 5.1 Tue 9:30 A 053

Strain-modulated defect engineering of two-dimensional materials — •Prosun Santra[1], Sadegh Ghaderzadeh[2], Mahdi Ghorbani-Asl[1], Hannu-Pekka Komsa[3], Elena Besley[2], and Arkady Krasheninnikov[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]School of Chemistry, University of Nottingham, Nottingham, U.K. — [3]Microelectronics Research Unit, University of Oulu, Oulu, Finland.

We have studied the response to external strain of h-BN, graphene, $MoSe_2$, and phosphorene, four archetypal 2D materials, which contain substitutional impurities, using first-principles calculations. We find that the formation energy of the defect structures can either increase or decrease with bi-axial tensile strain, depending on the atomic radius of the impurity atom which can be larger or smaller than that of the host atom. Analysis of the strain maps indicates that this behavior is associated with the compressive or tensile local strains produced by the impurities that interfere with the external strain. The discovered trends are consistent across all studied 2D materials and are likely to be general. Our findings open up opportunities for combined strain- and defect-engineering to tailor the opto-electronic properties of 2D materials, and specifically, the location and properties of single-photon emitters.

DS 5.2 Tue 9:45 A 053

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

We investigate the effect of the twist angle on the proximity spin-orbit coupling (SOC) in graphene/niobium diselenide (Gr/NbSe2) heterostructures from first principles. The low energy Dirac cones of several different commensurate twisted supercells are fitted to a model Hamiltonian, allowing us to analyze the twist-angle dependency of the SOC in detail. This reveals the possibility to triple the Rashba SOC, when going from 0° to 30° twist angle. Furthermore, at a critical twist angle of 23° the in-plane spin structure acquires a significant radial component, enabling collinear charge-to-spin conversion. Analyzing the Dirac cone with respect to allowed Umklapp processes and orbital decomposition shines light on the observed twist angle dependencies. In addition, we evaluate the potential for (collinear and perpendicular) charge-to-spin conversion in such heterostructures within linear response theory. 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 5.3 Tue 10:00 A 053

Ultra-sensitive real-time detection of SARS-CoV-2 proteins with carbon nanomembrane/graphene field-effect transistor heterostructure — •Hamid Reza Rasouli[1], David Kaiser[1], Ghazaleh Eshaghi[1], Marco Reinhard[2], Alexander Rolapp[2], Dominik Gary[3], Katrin Frankenfeld[3], Thomas Weimann[4], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Institut für Mikroelektronik- und Mechatronik-Systeme gemeinnützige (IMMS GmbH), 99099 Erfurt, Germany — [3]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb GmbH), 99947 Bad Langensalza, Germany — [4]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany

This study presents a novel approach to detect SARS-CoV-2 proteins based on graphene field effect transistors (GFET) functionalized via the van der Waals assembly with carbon nanomembranes (N3-CNM) enabling immobilization of antibodies for specific detection of the S- and N-proteins. A distinctive aspect of this approach is the simultaneous measurements of 15 GFETs integrated on a single chip with an automatic microfluidic system, facilitating the reliability for measuring the binding responses. The results demonstrate a detection limit down to the attomolar range with a dynamic response of 5 orders of magnitude. Furthermore, successful multiplex detection of S-protein and N-protein is demonstrated. The presented methodology paves the way towards highly sensitive, rapid, specific and multiplex detection of targets in various antibody-antigen systems.

DS 5.4 Tue 10:15 A 053

Graphene meets the macroscopic world: structure-property relationships and intercalation — •Florian Fuchs[1,2,3], Fabian Teichert[1,2,3], Daniel Dick[1,2,3], and Jörg Schuster[1,2,3] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

We study graphene-based conductor materials to leverage the excellent electronic transport properties of graphene into the macroscopic world. In these conductor materials, the individual graphene flakes form a layered macrostructure. A network model has been developed to relate microscopic graphene flake properties to the resulting macroscopic transport properties. Different flake sizes, packing densities, and contact geometries can be studied with this approach.

In addition, the layered structure of graphene-based conductor materials enables further material tuning by intercalating suitable materials in-between the graphene layers. An overview over different ongoing investigations of such systems, which are driven forward by density functional theory, will be given. We discuss the impact of different intercalants, like metal atoms and small molecules, onto the structural and electronical properties.

15 min. break

DS 5.5 Tue 10:45 A 053

Spin injection and detection in fully two-dimensional van der Waals devices — •Jan Bärenfänger[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jonathan Eroms[1], Dieter Weiss[1], and Mariusz Ciorga[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]National Institute for Materials Science, Tsukuba, Japan

In recent years, two-dimensional (2D) materials have attracted considerable attention for spintronic applications due to their vast electrical and magnetic properties. Especially, graphene, with its long spin relaxation times, and ferromagnetic Fe_3GeTe_2 (FGT), with its sharp magnetic switching behaviour and Curie temperatures up to room temperature, are 2D materials that seem to be predestined for spintronic applications. In this work we report efficient out-of-plane spin injection and detection in an all 2D van der Waals heterostructure using only exfoliated 2D materials. We demonstrate the spin-valve and Hanle effects in the non-local transport configuration in a stack of FGT, hexagonal boron nitride (hBN) and graphene layers. FGT flakes form the spin-aligning electrodes necessary to inject spins into the graphene channel and subsequently detect them. The hBN tunnel barrier provides a high quality interface between the ferromagnetic electrodes and graphene, eliminating the conductivity mismatch problem, thus ensuring efficient spin injection and detection. Our results demonstrate that FGT/hBN/graphene heterostructures form a promising platform for realizing 2D van der Waals spintronic devices.

DS 5.6 Tue 11:00 A 053

Extended Hubbard model describing small multi-dot arrays in bilayer graphene — •Angelika Knothe[1] and Guido Burkard[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Confined quantum dot states are attractive for various applications, from qubits to store quantum information to simulating exotic quantum phases. Here, we set up and parametrize a Hubbard model for interacting quantum dots in bilayer graphene and study double dots as the smallest multi-dot system. We demonstrate the tunability of the spin and valley multiplets, Hubbard parameters, and effective exchange constant by, e.g., gates and a magnetic field. For half-filling and large valley splittings, we derive and parametrize an effective Heisenberg

model for the quantum dot spins.

DS 5.7 Tue 11:15 A 053

Spin-Orbit Torque in Graphene / 1T-TaS_2 heterostructure — •Maedeh Rassekh[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia — [2]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia — [3]Faculty of Physics, University of Belgrade, Belgrade, Serbia — [4]Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

Spin-orbit torque (SOT) plays a critical role in enabling low-power and high-speed operation. In this study, we focus on investigating SOT acting on proximity-induced magnetization in graphene for the charge density wave ferromagnetic phase of 1T-TaS_2. Our findings reveal that the orientation and strength of the induced magnetization are influenced by the in-plane magnetization within the 1T-TaS_2 layer. Notably, alterations in the in-plane magnetization orientation within the 1T-TaS_2 layer led to the switching of charge-to-spin conversion mechanisms between the spin Hall effect and the Rashba-Edelstein effect. Furthermore, we extend our investigation to explore the impact of doping, particularly focusing on the vicinity of the Dirac point and hole-doped graphene. Our results highlight the importance of Fermi energy tuning for customizing spin transport properties in graphene/1T-TaS_2 heterostructures, which hold significant potential for future technological advancements. This work was supported by the APVV-SK-CZ-RD-21-0114, SASPRO 2 No. 945478, FLAG ERA JTC 2021 2DSOTECH, and IMPULZ IM-2021-42 projects.

DS 5.8 Tue 11:30 A 053

Proximity enhancement of Rashba angle in graphene/1T-TaS_2 heterostructures — •Martin Gmitra[1,2], Marko Milivojević[3,4], and Karol Szałowski[5] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [3]Institute of Informatics, Slovak Academy of Sciences, 84507 Bratislava, Slovakia — [4]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [5]University of Łódź, Faculty of Physics and Applied Informatics, Department of Solid State Physics, 90-236 Łódź, Poland

Van der Waals heterostructures provide unprecedented control of Dirac electronic states in graphene via proximity effects. In the talk, we present an electronic structure study of graphene/1T-TaS_2 heterostructure and show that the charge density wave phase in 1T-TaS_2 monolayer enhances significantly the Rashba angle in proximitized graphene. The Rashba spin-orbit coupling parameters can be further enhanced by applying a transverse electric field. We found also that the particular sandwich structures 1T-TaS_2/graphene/1T-TaS_2 trigger the Rashba angle to the $\pi/2$ limit relevant for specific charge-to-spin conversion utilizing collinear Rashba-Edelstein effect.

This work was supported by the APVV SK-CZ-RD-21-0114, FLAG ERA JTC 2021 2DSOTECH, IMPULZ IM-2021-42, and SASPRO 2 No. 945478 research grants.

DS 6: Thin Film Properties I

Time: Tuesday 9:30–12:45 Location: A 060

Invited Talk DS 6.1 Tue 9:30 A 060

Concerted electron-nuclear motion in polaron formation and exciton transfer — •Wolf Gero Schmidt — Universität Paderborn

Ab initio molecular dynamics calculations on (excited-state) potential energy surfaces obtained from constrained density-functional theory [1] provide deep insight into the concerted electron-nuclear motion of excited systems and allow for the quantitative modelling of the excitation dynamics [2]. This is demonstrated in my talk using two intriguing examples: (i) The formation of bound polarons in lithium niobate occurs on the femtosecond timescale [3] and modifies significantly the linear and nonlinear optical response [4]. (ii) The transfer of triplet excitons resulting from singlet fission in organic overlayers into Si solar cells is shown to be greatly accelerated by dangling-bond interface defects: The vibrations of Si surface atoms hosting the dangling bonds are associated with defect state energy changes that effectively shuttle the excitons across the interface [5].

[1] O Pankratov, M Scheffler, Phys. Rev. Lett. 75, 701 (1995).
[2] T Frigge et al., Nature 544, 207 (2017); CW Nicholson et al., Science 362, 821 (2018).
[3] M Krenz, U Gerstmann, WG Schmidt, Applied Physics A 128, 480 (2022).
[4] AL Kozub, A Schindlmayr, U Gerstmann, WG Schmidt, Phys. Rev. B 104, 174110 (2021).
[5] M Krenz, Verhandl. DPG (VI) 58, 572 (3/2023).

DS 6.2 Tue 10:00 A 060

Molecule adsorption at wz-Sc(x)Ga(1-x)N surfaces investigated by photo electron spectroscopy — •Fabian Ullmann[1,2], Abdul Qadir Shahbaz[1,2], and Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologie, Gustav-Kirchhoff-Straße 7, 98693 Ilmenau

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

DS 6.3 Tue 10:15 A 060

EXAFS Analysis of GeSn heteroepitaxial layers — •Sliman Gougam[1], Francesco De Angelis[2], Carlo Meneghini[2], Giovanni Capellini[1,2], and Marvin H. Zoellner[1] — [1]IHP-Leibniz-Institut für Innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Dipartimento di Scienze, Università Roma Tre, Viale G. Marconi 446 Roma 00146, Italy

There's considerable attention focused on GeSn epitaxial layers due to their promising use in advanced optoelectronic devices. GeSn epitaxial layers quality needs to be finely tuned through growth parameters, as the arrangement of Sn within the Ge crystal lattice may play a crucial role for its application. To study atomic short-range order around Sn in these films, X-ray Absorption Fine Structure (XAFS) spectroscopy is suitable due to its chemical selectivity and sensitivity to local structure. Here, we explore the short-range order of a series of Ge1-xSnx thin films grown on Ge/Si(001) virtual substrates using MBE. Sn K-edge XAFS spectra have been measured at ESRF where results show that Sn is coordinated to 4 Ge nearest neighbors. However, a distinct variation is observed in the next neighbor shell, where the analysis shows that the number of Sn next neighbors is larger than expected for a random distribution, suggesting a chemical ordering with higher Sn-Ge-Sn affinity, which in turn is influenced by growth conditions and film composition. Average modifications in local Sn arrangement among the samples revealed by XAFS, have been correlated with changes in structural properties probed by EDX analysis, which allows to reveal the dispersion of Sn throughout the layers.

15 min. break

DS 6.4 Tue 10:45 A 060

Controllable in-situ growth of nanostructured graphene on cubic-SiC/Si(001) wafers — •Victor Aristov[1,2], Olga Molodtsova[1], Sergey Babenkov[1,3], Dmitrii Potorochin[1,4], Dmitry Marchenko[5], Andrea Locatelli[6], Tevfik Onur Mentes[6], Alessandro Sala[6], and Alexander Chaika[7] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institut fuer Theoretische Physik, Universitaet Hamburg, 22607 Hamburg, Germany — [3]CEA-Saclay, 91190 Gif-sur-Yvette, France — [4]TU Bergakademie Freiberg, D-09599 Freiberg, Germany — [5]HZB für Materialien und Energie, D-12489 Berlin, Germany — [6]ElettraSincrotrone Trieste, I-34149 Basovizza, Trieste, Italy — [7]CRANN, School of Physics, Trinity College Dublin, Dublin 2, Ireland

The graphene grown on low-cost cubic-SiC/Si(001) wafers usually contains nanometer-sized domains with a few different lattice ori-

entations. Here we present the in-situ investigation of layer-by-layer graphene growth on such wafers. The measurements were performed using several methods: scanning tunneling microscopy with atomic resolution, low-energy electron microscopy (LEEM), high-resolution laterally-resolved X-ray photoelectron spectroscopy (micro-XPS), angle-resolved photoelectron spectroscopy (micro-ARPES), and micro low-energy electron diffraction (micro-LEED). The experimental data evidence the opportunity to control the local thickness of the graphene overlayer on the silicon carbide substrate in situ during UHV synthesis.

DS 6.5 Tue 11:00 A 060

Anatase-to-Rutile transformation in $CuTiO_2$ alloys — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Hao Lu[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Heinrich-Buff-Ring

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on float glass and quartz substrates by conventional rf-sputtering employing a TiO_2 ceramic target and Cu wires as Cu source. The surface morphology was measured by SEM. Systematic variations in film morphology were observed concomitant with alterations in the Cu content. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. For x = 23.5%, the minimum growth temperature for the rutile phase still can be as low as 200 °C. Transmission spectroscopy and ellipsometry reveal that the band gap of the $Cu_xTi_{1-x}O_2$ decreases with increasing x. Furthermore, we find that the morphology of the $Cu_xTi_{1-x}O_2$ thin films changes with increasing x. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

DS 6.6 Tue 11:15 A 060

Anisotropic strain relaxation in epitaxially constrained α-(Al,Ga)2O3 thin films on a-plane Al2O3 — •Anna Reis, Michael Hanke, Joao Marcelo Lopes, and Achim Trampert — Paul-Drude-Institut, Hausvogteiplatz 5, 10117 Berlin

Over the past two decades Ga2O3 in its thermodynamically stable β-phase has attracted large scientific interest due to its ultra-wide bandgap enabling the implementation of high-power electronic devices. Lately also the metastable trigonal α-phase of Ga2O3 has received growing attention. Being isostructural to α-Al2O3 ternary (Al,Ga)2O3 can be alloyed across the full compositional range allowing for bandgap engineering between 5.3 eV and 8.8 eV. In order to effectively design heterostructure devices detailed knowledge about strain formation and relief is of fundamental interest.

Thin α-(Al,Ga)2O3 films were epitaxially grown on lattice-mismatched a-plane Al2O3 via molecular beam epitaxy and probed in-situ by X-ray diffraction at the PHARAO facility at BESSY II. Grazing incidence diffraction patterns of the orthogonal (00.6) and (30.0) lattice planes reveal the in-plane strain dynamics of the interface. In the first monolayers the (Al,Ga)2O3 epilayer is found to be fully pseudomorphic whereas afterwards a partially relaxed layer is formed on top. Within deposition of the first 10-15 nm in-plane compressive strain accumulates preferably along the [100]-direction whilst along [001] strain is relieved exposing the anisotropy of the strain relaxation dynamics [A. Reis et al. Appl. Phys. Lett. 123, 122102 (2023)].

15 min. break

DS 6.7 Tue 11:45 A 060

Determination of Material Compositions from Strain Measurements in Scanning Transmission Electron Microscopy — •Frederik Otto, Laura Niermann, Tore Niermann, and Michael Lehmann — Technische Universität Berlin, Germany

Scanning Transmission Electron Microscopy (STEM) offers atomic-scale resolution for strain analysis by scanning a focused electron probe across a sample and evaluating the spacing between Bragg discs of the resulting electron diffraction patterns at each beam position. These Bragg discs contain features of multiple electron scattering, manifesting as patterns within the diffraction disc. While these patterns contain 3D scattering information, they can compromise the precise detection of diffraction discs' positions. To address this, a common strategy for achieving high-precision strain measurements involves utilizing a precessing electron beam, effectively averaging over multiple patterns.

In this study, rather than disregarding the effects of multiple electron scattering, we focus on carefully evaluating variations in the patterns. A comparative analysis of measured diffraction discs and simulations reveal that these variations originate from deformations appearing at the TEM lamella's surface. These deformations arise as a consequence of stress relaxation in a strained sample during the preparation process. Therefore, this effect is indicative of the strain in the sample (here: the (Al,Ga)N/GaN interface) and thus provides insights into the material's composition. Consequently, we demonstrate a novel method for deducing the composition of layered structures through a single STEM measurement of the strain at the interfaces.

DS 6.8 Tue 12:00 A 060

Precision Through Precession: Enhanced Accuracy of Strain Investigations in Scanning Transmission Electron Microscopy — •Rahel Specht, Frederik Otto, Laura Niermann, Tore Niermann, and Michael Lehmann — Technische Universität Berlin, Germany

In semiconductor development, strain engineering plays a pivotal role, for example in enhancing piezoelectrical effects in AlGaN quantum wells. With ever decreasing device sizes, knowledge of interacial strain at high spatial resolution is an important feedback for the manufacturing process. Scanning Transmission Electron Microscopy (STEM) is capable of resolving the local lattice spacing with nanometer resolution by scanning a focused electron probe over the sample and evaluating the distance of diffraction discs at each respective beam position. However, due to multiple electron scattering and subsequent interference, intensity variations appear in the resulting diffraction discs. These variations hinder the precise detection of the disc's position in the diffraction pattern. In this work, we employ a precessing electron beam to map the position-dependent measurement of lattice spacing of (Al,Ga)N in GaN. Precessing the electron beam effectively averages multiple diffraction patterns, resulting in a more uniform intensity distribution in the diffraction discs. While larger precession angles enhance the precision of disc detection, due to microscope aberrations, higher precession angles also lead to a reduction in spatial resolution. Therefore, we aim to outline a pathway to determining optimal settings for high-resolution strain measurements at heterointerfaces in STEM.

DS 6.9 Tue 12:15 A 060

Spiral and pyramid like structures in solvent prepared crystalline organic C13-BTBT thin films — •Fabian Streller[1], Manuel Johnson[1], Mingjian Wu[2], Erdmann Spiecker[2], and Rainer Fink[1] — [1]Friedrich Alexander Universität Erlangen Nürnberg (FAU), Department Chemistry & Pharmacy — [2]Friedrich Alexander Universität Erlangen Nürnberg (FAU), Department Materials Science und Engineering

The demand for high quality organic thin films for electronic applications is steadily increasing. In OLEDs, OFETs, or sensorics devices, their light weight, flexibility, chemical tunability, and large area preparation makes organic semiconductors valuable resources. Saturated solutions of many aromatic molecules may lead to the formation of large-area crystalline 2D organic film at the solvent-water interface driven by the π-π-interactions for molecular self-organization. In rare cases we observe spiral and pyramidal structures. Excitingly, 3D structures in solvent prepared α-,ω-Hex-6T-Hex show uniform azimuthal rotations in subsequent layers. Here we extend these studies onto mono-substituted C13-BTBT. The interaction towards the water and thus the ratio of intra- vs. interlayer interactions was modified by water surfactants. Compared to previous results, the 3D structures are more extended. Complementary microscopic (AFM, KPFM, TEM, 4D-SCEM) and spectroscopic probes were applied to gain further insight into structure-property relationships and the origin of specific 3D structures. The research is funded by the BMBF (contract 05K22WE2).

DS 6.10 Tue 12:30 A 060

Detailed Microstructure and the Influence of Post-Treatment on CVD TiAlN Wear-Resistant Coatings — •Monica Mead[1], Olof Bäcke[2], Dirk Stiens[3], and Mats Halvarsson[2] — [1]Institute for Materials Science, University of Stuttgart, Germany —

[2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [3]Walter AG, Tübingen, Germany

The suitable properties of cubic TiAlN have led to its importance as wear-resistant coating for cutting tools. Preparation by chemical vapour deposition (CVD) has enabled deposition with Al contents above 90 at.% while limiting formation of undesired hexagonal TiAlN. Despite intensive research on the growth of CVD TiAlN coatings, there is no comprehensive understanding of the growth mechanism and intricate microstructure. In addition, research on the effect of blasting on the stress state of wear-resistant coatings is considerable, while the effect on the microstructure is less well studied.

In this work, the microstructure of nano-lamellar low-pressure CVD TiAlN coatings on cemented carbide substrates and the influence of blasting is investigated by scanning electron microscopy (SEM), scanning transmission electron microscopy (STEM) and transmission Kikuchi diffraction (TKD). Two distinct morphologies are observed and connected to specific grain orientations. Furthermore, the proposed growth mechanism suggests an influence of the detailed microstructure on the surface reaction kinetics leading to varying Al/Ti ratios. Blast-treatment of the hard TiAlN coatings introduces plastic deformation, where an influence of the grain orientation is observed.

DS 7: 2D Materials and their Heterostructures III

Time: Wednesday 9:30–11:45 Location: A 053

DS 7.1 Wed 9:30 A 053

Two-dimensional platinum chalcogenides: controlling stoichiometry for electronic applications — •Mahdi Ghorbani-Asl and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

Among layered materials, platinum chalcogenides have received great attention due to their peculiar physical properties. The strong layer-dependent electronic properties cause the opening of a band gap in monolayer $PtTe_2$, while the system otherwise is (semi)metallic. Here we show that starting with $PtTe_2$ films, other compositions such as Pt_3Te_4 and Pt_2Te_2 can be obtained by a postgrowth desorption of tellurium or vapor-deposited Pt atoms. The experiments combined with DFT calculations provide insights into these transformation mechanisms and the stabilization of the new phases. The partially converted monolayer flakes exhibit $PtTe_2$-Pt_2Te_2 heterojunctions, which enable the formation of the in-plane semiconductor-metal interface. We further studied the electronic structure of edges and point defects in $PtSe_2$ monolayer where metallic 1D states with spin-polarized bands were found. In addition to stoichiometry, combining different Pt-chalcogenides in the form of vertical heterostructures provides an additional degree of engineering of materials properties. Our results showed the variation of the interlayer interaction within the moiré structure locally modulates the electronic structure of $PtSe_2/PtTe_2$ heterostructures.

DS 7.2 Wed 9:45 A 053

Classification of layered chalcogenides: explaining their mineral diversity in the Earth's crust — •Alexander Kiehn[1], Carl-Friedrich Schön[2], Christian Stenz[2], Sebastian Gruner[2], Jan Köttgen[2], Jean-Yves Raty[3], and Matthias Wuttig[1,2] — [1]PGI 10, Forschungszentrum Jülich; Johnen-Straße, 52428 Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University; Sommerfeldstraße 14, 52056 Aachen, Germany — [3]CESAM, Université de Liège; Quartier Agora, Allée du six Août 19, 4000 Liège, Belgium

Layered or 2D chalcogenides are a material class with exceptional properties enabling manifold applications. Using quantum-chemical calculations, these materials can be classified into three families based on the distance between layers as well as the translation energy parallel to these layers. Containing many TMDCs, the largest group of layered chalcogenides forms van der Waals bonds across the gaps, which are characterized by large atomic spacings, small translation energies and weak interlayer bonding. Conversely, two other groups are identified by shorter interlayer gaps, larger translation energies and significantly stronger interlayer coupling. For several compounds, like Bi2Te3, these properties can be attributed to their special bonding mechanism. Notably, when combining compatible layer types into varying stacks, this large coupling allows for an energy hierarchy of interlayer bonding. This explains the rich phase diagrams of heavy p-block elements, like Sb, As, Bi and Te, and is also mirrored in their anomalously high mineral diversity. The evidence for strong interlayer coupling is supported by electron microscopy and laser-assisted bond-rupture experiments.

DS 7.3 Wed 10:00 A 053

Misfit Layer Compounds as Ultratunable Field Effect Transistors: From Charge Transfer Control to Emergent Superconductivity — •Ludovica Zullo[1,2], Giovanni Marini[1], Tristan Cren[2], and Matteo Calandra[1,2,3] — [1]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [2]Sorbonne Université, CNRS, Institut des Nanosciences de Paris (INSP), UMR7588, F-75252 Paris, France — [3]Graphene Labs, Fondazione Istituto Italiano di Tecnologia, Via Morego, I-16163 Genova, Italy

Misfit layer compounds (MCLs) are heterostructures composed of rocksalts units stacked with few layers transition metal dichalcogenides (TMDs) [1]. Because of the lattice mismatch and chemical bonding between constituents, bulk MLCs behave similarly to mono and bi layer TMDs, making it quasi-2D systems. In this work [2], by means of density functional theory, we show that misfits behave as a periodic arrangement of ultra-tunable field effect transistors with 2D features. We demonstrate how the charge injection into the TMD layers can be controlled by the chemistry of the rocksalt which always acts as electron donor. Finally, we establish a strategy to design emergent superconductivity and demonstrate its applicability in $(LaSe)_{1.27}(SnSe_2)_2$, showing that superconductivity can emerge in MLCs formed by assembling non-superconducting rocksalts and TMDs.

[1] Gerrit Wiegers, Progress in Solid State Chemistry 24, 1 (1996)
[2] Ludovica Zullo, Giovanni Marini, Tristan Cren, Matteo Calandra Nano Lett. 2023, 23, 14, 6658-6663 (2023)

DS 7.4 Wed 10:15 A 053

Direct visualization of stacking-selective self-intercalation in epitaxial $Nb_{1+x}Se_2$ films — Hongguang Wang[1], •Jiawei Zhang[1], Chen Shen[2], Chao Yang[1], Kathrin Küster[1], Ulrich Starke[1], Hongbin Zhang[2], Dennis Huang[1], Peter A. van Aken[1], and Hidenori Takagi[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64289 Darmstadt, Germany

Two-dimensional (2D) van der Waals (vdW) materials are particularly intriguing due to the rich tuning possibilities offered by stacking 2D layers or introducing intercalants into the vdW gaps. However, current knowledge of the interplay between stacking polytypes and intercalation is limited by macroscopically averaged probes. Here, using atomic-resolution electron energy-loss spectroscopy in a scanning transmission electron microscope, we directly visualize a stacking-selective self-intercalation phenomenon in the transition-metal dichalcogenide (TMDC) material $Nb_{1+x}Se_2$: In epitaxial $Nb_{1+x}Se_2$ films with both the parent 180° stacking and additional 0°-stacked phases, the excess Nb atoms are predominantly found between the 180°-stacked layers. The 0°-stacked layers arise as a means of staggering the intercalants, *i.e.*, to increase their interlayer separation, rather than to accommodate the intercalants themselves, as has been previously suggested. Our results not only provide an updated microscopic understanding of $Nb_{1+x}Se_2$, but also prospects for engineering the functionality of TMDCs via stacking-selective self-intercalation.

15 min. break

DS 7.5 Wed 10:45 A 053

Nontrivial magnetic helical states and electric polarization in NiI_2 monolayer — •Juraj Mnich[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia

A monolayer of NiI_2 enriches a small group of 2D multiferroic materials possessing unique magnetic and electric polarization properties.

Trigonal crystal symmetry and the interplay between spatially dependent ferromagnetic and antiferromagnetic exchange interactions, along with strong spin-orbit coupling, give rise to complex helical magnetic states. The helical state can be described by a wave propagation vector and a plane in which magnetic moments rotate. We studied several magnetic helical states using first-principles calculations. We found that the alignment of magnetic moments gives rise to unexpected electric polarization for a proper screw helical state. We also studied the interplay between the helical states and electric polarization in the NiI_2 bilayer and we speculate that an in-plane bias voltage can induce rotation of the helical state via spin-transfer torque, dragging its phase and switching the wave propagation vector, reflecting in electric polarization reversal.

This work was supported by the APVV-SK-CZ-RD-21-0114, FLAG ERA JTC 2021 2DSOTECH, and IMPULZ IM-2021-42 research grants.

DS 7.6 Wed 11:00 A 053

Electronic structure of intercalated α-$NbSi_2N_4$ and α-$TaSi_2N_4$ monolayers and their van der Waals heterostructures — •Timon Moško[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Juraj Mnich Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia

Recent DFT studies of monolayer materials promote intercalated MA_2Z_4 monolayers as versatile atomically thin materials with a wide spectrum of physical properties. In the talk, we present a first-principles study of the electronic structure of α-$NbSi_2N_4$ and α-$TaSi_2N_4$ monolayers, as well as their heterostructure. We investigate mechanical stability, charge density wave formation, electronic susceptibility, and magnetic order. We found that the Hubbard on-site on metallic atoms M drives the α-$NbSi_2N_4$ from a magnetic conductor to a magnetic insulator and α-$TaSi_2N_4$ from a non-magnetic Eliashberg superconductor to a magnetic insulator. Magnetic ground state properties were analyzed using a classical Heisenberg model, providing insights into exchange integrals, magnetocrystalline anisotropy, and critical transition temperatures. Proximity-induced effects in α-$NbSi_2N_4$ / α-$TaSi_2N_4$ heterostructure uncover lead to the doping effect and emergence of the narrow Ta d_{z^2} hole pocket at the Brillouin zone center susceptible to suggesting its potential as a hybrid system for controlling spin and thermal transport under a transverse electric field.

This work was supported by the APVV SK-CZ-RD-21-0114, FLAG ERA JTC 2021 2DSOTECH, and IMPULZ IM-2021-42 grants.

DS 7.7 Wed 11:15 A 053

Quasiparticle Interference patterns of monolayer $NbSe_2$, an Ising superconductor with Rashba spin-orbit coupling — •Jozef Haniš[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [2]Institute of Informatics, Slovak Academy of Sciences, 84507 Bratislava, Slovakia — [3]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [4]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia

A monolayer of $NbSe_2$ is a 2D superconductor with unconventional Ising pairing that sustains tremendous in-plane magnetic fields. In a realistic setup, the presence of the substrate triggers the Rashba spin-orbit coupling in $NbSe_2$ and an in-plane spin texture in the superconducting material. It was experimentally suggested that such a system can host both nodal and nematic superconductivity, motivating us to theoretically construct all the possible types of singlet and triplet superconducting pairings allowed. Furthermore, we calculate the quasiparticle interference (QPI) patterns in the limit of a single scalar impurity. We found pronounced differences in the QPI patterns of the superconducting pairing functions constructed using the group-theoretical approach, suggesting that the QPI spectrum analysis can provide valuable insights into the potential understanding of the unconventional pairing when confronted with the scanning tunneling spectroscopy measurements.

This work was supported by the IMPULZ IM-2021-42, APVV SK-PL-21-0055, and SASPRO 2 No. 945478 research grants.

DS 7.8 Wed 11:30 A 053

Visible-Light-Active 2D Single-Layered g-C_3N_4-TiO_2 Thin Film Photocatalysis — •Narmina O. Balayeva[1,2], Bowei Zhan[1,2], Yevhenii Havryliuk[1,2], Oleksandr Selyshchev[1,2], and Dietrich R.T. Zahn[1,2] — [1]Institute of Physics, TU Chemnitz, Reichenhainer Str. 70 — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Rosenbergstr. 6

Recently, the interest in the application of atomically thin 2D "graphene-like" layered graphitic carbon nitride (g-C_3N_4) for visible-light efficient photocatalysis has significantly increased. This work demonstrates the fabrication of thin film heterostructures of single-layered g-C_3N_4 (SLGCN) and the anatase TiO_2. After obtaining SLGCN from base-assisted exfoliation of bulk g-C_3N_4, the films were prepared using spray coating with 1, 3, and 5 cycles on p-type Si(100) substrates. Subsequently, a colloidal TiO_2 solution was deposited using spin coating and annealed at 500 °C to form the anatase polymorph. Secondly, the powder of SLGCN was mixed with the colloidal TiO_2 solution at different relative weight percentages (5-50 wt%) and deposited using spin coating followed by the same annealing procedure. The morphology, structural, and optical properties of SLGCN and SLGCN-TiO_2 are characterized by XRD, AFM, SEM, and spectroscopic techniques such as UV-vis, Raman, FTIR, and ellipsometry. Finally, the photocatalytic degradation of acetone and CO_2 reduction was studied using an FTIR-based gas photo-reactor chamber equipped with 1 mW/cm^2 LED with different wavelengths.

DS 8: Thin Film Properties II

Time: Wednesday 9:30–12:30 Location: A 060

DS 8.1 Wed 9:30 A 060

Vacancy like defects in Cd3As2 — •Maciej Oskar Liedke[1], Anthony Rice[2], Maik Butterling[1], Eric Hirschmann[1], Nancy M. Haegel[2], Kirstin Alberi[2], and Andreas Wagner[1] — [1]Institute of Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, Dresden 01328, Germany — [2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Cd3As2 is a three-dimensional topological semimetal which can be transformed into exotic phases, e.g., Weyl semimetals, topological superconductors, or axion insulators. Using epitaxy provides an avenue for varying and controlling point defects during Cd3As2 growth. The knowledge of vacancy defects is essential for interpretation of electron transport behavior and guides growth efforts to develop materials with low defect concentrations. Point defects in Cd3As2 epilayers grown by molecular beam epitaxy with varying As/Cd flux ratios are probed by positron annihilation spectroscopy. We show that lower As/Cd flux ratios produce higher concentrations of point defects. Remarkably, the measurements indicate that the average defect size is larger than a monovacancy and vacancy complexes dominate [Rice et al. APL Mater 11, 061109 (2023)]. The evolution of defect microstructure as a function of temperature will be discussed as well.

DS 8.2 Wed 9:45 A 060

Towards high-throughput studies of gradient multi-component thin films — •Dmitry Lapkin, Alexander Gerlach, Alexander Hinderhofer, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Progress in the development of modern functional materials is indispensable for technological progress. In many cases, these materials are complex multi-component systems, with a rather non-trivial dependence of the properties on composition. A typically non-linear and non-monotonic composition dependence makes it mandatory to investigate the resulting properties with many points on the composition axis, and ideally within one given sample to ensure comparability, calling for suitable sample preparation techniques.

An example of such a preparation technique relevant for applications is organic molecular beam deposition (OMBD) of organic semiconductor thin films. A deposition chamber, recently developed in our group, makes it possible to overcome unintentional variations in deposition conditions for different samples and, importantly, to obtain a film with a composition gradient in one run.

In this work, we demonstrate the preliminary results of gradient two-component film deposition and how the spatial resolution of mod-

ern sample characterization methods can be effectively converted into compositional resolution using such gradient films. In combination with arising machine learning-based on-the-fly data treatment methods, this opens up horizons for high-throughput studies of the structure and properties of multi-component thin films.

DS 8.3 Wed 10:00 A 060

Structural and magnetic anisotropy in YBa2Cu3O7/ La0.67Sr0.33MnO3 bilayer film on SrTiO3 substrate — •Ankita Singh, Sawani Datta, Ram Prakash Pandeya, Srinivas C. Kandukuri, and Kalobaran Maiti — Department of Condensed Matter Physics & Material Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai-400005, India

We study the magnetic properties and emergence of superconductivity in YBa2Cu3O7 (YBCO)/ La0.67Sr0.33MnO3 (LSMO) heterostructures. Bilayer films of superconducting layer, YBCO and ferromagnetic layer, LSMO were grown on SrTiO3 (STO) (001) substrate using a home built ultrahigh vacuum (UHV) pulsed laser deposition (PLD) system. Magnetization data at 100 K as a function of applied field shows ferromagnetic behaviour due to the LSMO layer. Cooling below 100 K leads to superconductivity in this material; the onset of superconductivity occurs at a temperature TC(onset) of 86 K for Hext*c (in-plane) and Hext || c (out-of-plane) under 100 Oe applied field. In-plane magnetic measurements show significant suppression of diamagnetic behaviour as compared to the out-of-plane measurements. The susceptibility signals are higher for the out-of-plane direction. Such strong anisotropy in magnetism below the transition temperature reveal complex interplay of magnetism and superconductivity in this system and calls for further study in this direction.

DS 8.4 Wed 10:15 A 060

Calcium Made Interesting — •Kai Bröking[1,2,3], Stephan Brückner[1], Daniel Tasche[1,2], and Christoph Gerhard[1,4] — [1]Hochschule für Angewandte Wissenschaft und Kunst, Göttingen, Germany — [2]Technische Universität Clausthal, Fakultät für Natur- und Materialwissenschaften, Clausthal-Zellerfeld, Germany — [3]Max-Planck-Institut für multidisziplinäre Naturwissenschaften, Göttingen, Germany — [4]School of Industrial and Information Engineering, Politecnico di Milano, Milano, Italy

During manufacturing, optical glass components come into contact with a variety of process agents. An exchange between the glass and these chemical compounds leads to the accumulation of some of their ingredients in surface and sub-surface defects, and, by diffusion, in the glass itself [1]. On the other hand, a depletion of glass constituents near the glass surface takes place as well. As can be expected, these processes lead to unwanted changes in glass properties near the surface [2] and may facilitate its deterioration. We investigate both depletion and accumulation of metal ions near the surfaces of multi-component glasses and explore the scaling behaviours of the transport processes involved.

[1] Gerhard &al., Applied Surface Science Volume 537, 30 January 2021, 147984, doi:10.1016/j.apsusc.2020.147984

[2] Gerhard, Köhler, Opt Mater Expr Vol. 12, Issue 9, pp. 3658-3666 (2022), doi:10.1364/OME.458227

15 min. break

DS 8.5 Wed 10:45 A 060

Study of self-organized structures at metal-organic interface In/CuPcFx — •Olga Molodtsova[1], Dmitrii Potorochin[1,2], Sergey Babenkov[1,3], Serguei Molodtsov[2,4], Anna Makarova[5], Dmitry Smirnov[6], and Victor Aristov[1] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]TUBergakademie Freiberg, D-09599 Freiberg, Germany — [3]CEA-Saclay, 91190 Gif-sur-Yvette, France — [4]Europian XFEL GmbH, D-22869 Schenefeld, Germany — [5]Institute of Chemistry and Biochemistry, Free University of Berlin, D-14195 Berlin, Germany — [6]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany

The start and development of molecular electronics has attracted particular attention to molecular semiconductors such as metal phthalocyanines. They have unique properties and are technologically advanced in production. Using ultrathin films as a matrix, it is possible to create metal-organic composites containing metal nanoparticles that self-organize in an organic matrix. The technologies for creating the described nanocomposites are quite simple and relatively cheap; therefore, such materials can find a prominent place in practical applications in various electronic devices. However, despite the growing interest in hybrid systems, numerous questions about their properties and the processes occurring during their formation remain unanswered. For example, interfacial phenomena can radically change the electronic properties of organic wide-gap matrices.

DS 8.6 Wed 11:00 A 060

Stability and Elasticity of Ultrathin Sphere-Patterned Block Copolymer Films — •Le Qiao[1], Daniel A. Vega[2], and Friederike Schmid[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D55099 Mainz, Germany — [2]Instituto de Física del Sur (IFISUR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina

Sphere-patterned ultrathin block copolymers films are potentially interesting for a variety of applications in nanotechnology. We use self-consistent field theory to investigate the elastic response of sphere monolayer films with respect to in-plane shear, in-plane extension and compression deformations, and with respect to bending. The relations between the in-plane elastic moduli is roughly compatible with the expectations for two-dimensional elastic systems with hexagonal symmetry, with one notable exception: The pure shear and the simple shear moduli differ from each other by roughly 20%. Even more importantly, the bending constants are found to be negative, indicating that free-standing block copolymer membranes made of only sphere monolayer are inherently unstable. Our results are discussed in view of experimental findings.

DS 8.7 Wed 11:15 A 060

Defect break-down in systematically disordered Cr_2AlC — •Joao S. Cabaco[1,6], Maciej O. Liedke[2], Javier Pablo-Navarro[3,4], Fabian Ganss[1], Cesar Magen[3], Manuel R. Ibarra[3,4], Ulrich Kentsch[1], Maik Butterling[2], Andreas Wagner[2], Jurgen Lindner[1], Jurgen Fassbender[1,5], Christoph Leyens[6], Richard Boucher[6], and Rantej Bali[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [2]Institute of Radiation Physics, HZDR, Germany — [3]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain — [4]Laboratory of Advanced Microscopies, University of Zaragoza, Spain — [5]Institute of Solid State and Materials Physics, TU Dresden, Germany — [6]Institute of Materials Science, TU Dresden, Germany

The presence of open-volume defects, such as vacancies, can influence the structural, magnetic, and transport properties. This study uses ion irradiation to investigate the evolution of defects in MAX-phase Cr_2AlC. Thin-films of 50 nm and 500 nm were irradiated at increasing fluences, using both inert ions and transition metal ions. Through the combined use of positron annihilation and *ab-initio* simulations, it was possible to distinguish different types of defects, determine their size and concentration. Large clusters of 9-15 vacancies, originally present in the as-grown films, transform into Al mono-vacancies and Cr-Al di-vacancies upon ion irradiation. Furthermore, an overall reduction in open-volume defect concentration and size due to irradiation was observed. **Grant:** (DFG) TRANSMAX no. 456078299.

15 min. break

DS 8.8 Wed 11:45 A 060

Phase-Selective Epitaxy of Trigonal and Orthorhombic Bismuth Thin Films on Si (111) — •Xiao Hou[1], Abdur Rehman Jalil[2], Peter Schüffelgen[2], Claus Michael Schneider[1], Lukasz Plucinski[1], and Detlev Grützmacher[2] — [1]Peter-Grünberg-Institute (PGI-6) — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Over the past decades, the growth of Bi thin films has been extensively explored due to their potential applications such as thermoelectrics, ferroelectrics, and recently in topological and neuromorphic areas. The strong spin-orbit coupling renders some Bi allotropes topologically non-trivial [1], offering opportunities to explore topological devices. Besides, due to its thermal instability, Bi is a suitable candidate for phase-change and low-power neuromorphic applications. Despite significant research efforts, achieving reliable and controllable growth of high-quality Bi thin-film allotropes has remained a challenge [2].
This study is dedicated to achieve well-controlled high-quality growth of Bi epilayer on Bi-terminated Si (111) 1×1 surfaces using MBE. With

systematic growth, this work yields a phase map that demonstrates the realization of trigonal, orthorhombic, and pseudo cubic thin-film allotropes of Bi. In-depth characterization through XRD techniques and STEM analysis provides a comprehensive understanding of phase segregation, phase stability, phase transformation, and phase-dependent thickness limitations in various Bi thin film allotropes.
[1] Jalil A R. PhD thesis. RWTH Aachen, Germany (2022). [2] Jalil A R, Hou X, et al. Nanomaterials (2023).

DS 8.9 Wed 12:00 A 060

Design of a polymeric thin film for 2D material printing — •Sebastiaan Haartsen[1], Pantelis Bampoulis[1], Harold Zandvliet[1], Johannes Aprojanz[1,2], Inga Wille[2], and Harald Jasper[2] — [1]University of Twente — [2]Actega Metal Print GmbH

In this talk, we present a method of printing 2D materials based on flexographic printing. In this method, 2D materials are transferred to a polymeric surface. Using additives, we show that the adhesive properties of a polymeric thin film can be modified to enhance the transfer of the 2D material.

Crossectional atomic force spectroscopy together with surface spectroscopy allows for a greater understanding of the enhancements caused by the additive. Using low concentrations of the additive, we record a segregation of the additive towards the surface of the thin film, shown by an increase in the adhesive force and energy. Increasing the concentration of the additive from 1 to 10$wt\%$ enhances the adhesive properties at the surface while concentrations higher than 10$wt\%$ reduce the adhesive properties. Above 10

Results from this research are used for the design of a polymeric thin film suitable for 2D material printing.

DS 8.10 Wed 12:15 A 060

Atomic imaging of the critical nucleus size of multilayer hexagonal ice growth — •Dong Guan, Tiancheng Liang, Zixiang Yan, Li-Mei Xu, En-Ge Wang, and Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China

Multilayer water ice growth is widespread and plays a significant role in various natural phenomena. An essential aspect of water ice growth is the elusive nature of the critical ice nucleus, attributed to its transient and delicate characteristics. We present the precise atomic size of the critical ice nucleus in hexagonal water ice (ice Ih) through the utilization of qPlus-based cryogenic noncontact atomic force microscopy (NC-AFM) equipped with a CO-terminated tip. Freezing samples during the growth process allows us to capture the intermediate structures involved in the growth of Ih ice. Our investigation reveals that pentamers and hexamers are the most prevalent intermediate structures, and their combination gives rise to the 3-5 cluster, which we define as the critical ice nucleus. Combined with density functional theory, we might show that the structure alteration of the 3-5 cluster results in the formation of a new core for Ih ice. This new core can expand by incorporating additional water molecules along its periphery. This research is the first achievement in elucidating the exact atomic structure of a critical ice nucleus in water. It provides valuable insights into the water freezing process and holds the potential for application to other nucleation processes.

DS 9: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides I (joint session DS/MM/O)

MXenes, two-dimensional transition metal carbides, nitrides and carbonitrides, constitute one of the most rapidly growing class of 2D materials. Discovered in 2010, they have demonstrated exceptional physical, chemical, and electronic properties leading to potential applications in various fields, such as energy storage, catalysis, electromagnetic interference shielding, sensing, and biomedicine. The fundamental physical properties of MXenes are governed by their chemical composition and great research efforts are currently devoted to expanding the range of existing MXenes by tuning their stoichiometry, morphology and surface chemistry as well as adding tailored defects that can bring new functionalities. In this Focus Session, new developments related to MXene synthesis and characterization will be presented. The fundamental physical properties and interfacial processes correlated with MXene surface chemistry, defects and interlayer confinement will be discussed.

Organizers:

Dr. Tristan Petit, Head of the Young Investigator Group Nanoscale Solid-Liquid Interfaces, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Prof. Vincent Mauchamp, Institut Pprime, CNRS-Université de Poitiers-ISAE ENSMA, Poitiers, France

Time: Wednesday 15:00–17:00 Location: A 053

Introduction Focus Session on MXene - V. Mauchamp & T. Petit

Invited Talk DS 9.1 Wed 15:15 A 053

Sustainable synthesis of MXenes and their precursors — •Jesus Gonzalez-Julian[1], Nima Amousa[1], and Filipa Oliveira[2] — [1]Chair of Ceramics, Institute of Mineral Engineering (GHI), RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Inorganic Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic

Synthesis of MXenes is typically performed using HF - or forming in-situ HF through the reaction between LiF and HCl, but this chemical etching presents some limitations. HF is highly corrosive and toxic, requiring specific safety regulations, and the chemical etching is highly exothermic, limiting the amount of MXenes that can be produced in the range of grams. These two points are hindering the transfer of MXenes to real applications, despite the excellent properties of these 2D materials. Consequently, new synthesis processes are required to overcome these problems. In this work, we will present a novel sustainable synthesis route for the synthesis of the precursors (MAX phases) and the chemical etching, which is referenced as Molten Salt Shielded Synthesis or MS3. MS3 is carried out at lower temperatures than conventional synthesis routes, in air instead inert atmospheres, and does not require any milling step to obtain fine and loose powders.

DS 9.2 Wed 15:45 A 053

Tuning the molten salt etching process by in situ XRD — •Julian T. Müller, Aleksander Gurlo, and Maged F. Bekheet — Technische Universität Berlin, Faculty III Process Sciences, Institute of Material Science and Technology, Chair of Advanced Ceramic Materials, Straße des 17. Juni 135, 10623 Berlin, Germany

MXenes, whose properties are mainly defined by their chemical composition and surface terminations, could be synthesized by etching an A element (A = Al, Si, etc.) from the parent MAX phase using hydrofluoric acid. This acid is of high risk to human health and leads to fluorine terminations on the surface of MXene, which are difficult to alter and may be detrimental for certain applications, e.g. electrodes in different battery systems. Etching via molten salt formation offers an alternative, less harmful way. By sophisticated selection of salts, it is possible to adjust the surface terminations and pave the way for a new generation of tailored MXenes. Gaining insight into the molten salt etching process and tuning its process parameters such as temperature,

duration, and precursor ratio are keys to ensuring a qualitative MXene and saving time, energy, and cost. To support this, we are currently establishing an in situ XRD setup at the Advanced Light Source of the Lawrence Berkeley National Laboratory. It will allow measurements under various gas atmospheres up to 1450 °C and 50 bars, including a vapour phase. In the first molten salt etching experiments, we successfully gained knowledge on the etching onset, duration, and phase composition. With this measurement setup, the synthesis of MAX phases and many MXene and salt combinations await to be explored.

DS 9.3 Wed 16:00 A 053

Preparation of Magnetic MXenes by Fe intercalation — Tim Salzmann[1], Hanna Pazniak[2], Thierry Ouisse[2], Fabrice Wilhelm[3], Andrei Rogalev[3], Ralf Meckenstock[1], Ivan Tarasov[1], Michael Farle[1], and •Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France — [3]European Synchrotron Radiation Facility, Grenoble, France

Yet, the success of generating magnetic MXenes remains very limited since Fe, Co or Ni are incompatible with MAX phase precursors. We present an alternative approach to master magnetic properties of 2D MXenes by intercalating Fe into $Ti_3C_2T_x$ MXene thin films on Si/SiO_2 in UHV conditions. Annealing of bare MXenes at T = 1023 K removes -F, -Cl and -OH. The intercalation of Fe is studied by depositing a 6 nm film on top of the MXenes and subsequent annealing. XRD shows an increase of the interplanar spacing between MXene sheets of 0.16 ± 0.02 nm. XPS and XANES reveal that Fe remains metallic and Fe diffuses 30 nm deep into the multilayers while MXenes keep intact. We study the magnetic properties by VSM and FMR. VSM suggests a new magnetic phase with $M_S = 660 \pm 80$ kA/m and a Curie temperature of 485 K while angular-dependent FMR at 9 GHz and 300 K shows two ferromagnetic and one paramagnetic signals, which we address to the remaining Fe on top and the intercalated Fe in form of quasi 2D disks and isolated Fe ions. Funded by DFG (530103526). Support by CRC/TRR 270 (405553726) is acknowledged.

DS 9.4 Wed 16:15 A 053

synthesis and characterization of 2D Mo/Ti solid solutions based MXene for hydrogen evolution reaction in alkaline media. — Lola Loupias[1], Claudia Morais[1], Sophie Morisset[1], Christine Canaff[1], Zheming Li[1], Patrick Chartier[2], Vincent Mauchamp[2], Thierry Cabioc'h[2], Aurélien Habrioux[1], and •Stéphane Célérier[1] — [1]Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), Université de Poitiers, CNRS, F-86073 Poitiers, France — [2]Institut Pprime, UPR 3346 CNRS, Université de Poitiers, ISAE-ENSMA, BP 30179, 86962 Futuroscope-Chasseneuil Cedex, France

2D MXenes have gained an ever-increasing attention in various application fields. Their properties can be strongly tuned by modifying the M element in the Mn+1XnTx structure. Among them, Mo-based MXenes are beginning to be successfully explored in many areas. This work focuses on the synthesis and characterization of (Mo,Ti)n+1CnTx MXenes to understand their complex chemistry and to compare them with those of mono-metallic Mo2CTx and Ti3C2Tx. The potential of these materials as HER (hydrogen evolution reaction) catalysts is determined in alkaline medium. It is shown that Mo2Ti2C3Tx MXenes are a credible alternative to Mo2CTx MXenes since the surface properties of both MXenes are similar while their composition is quite different. Indeed, (Mo,Ti)n+1CnTx require lower temperatures and shorter time for the synthesis than for Mo2CTx, a great advantage from an industrial point of view. Finally, some avenues for improving the performance of MXenes for HER will also be described.

DS 9.5 Wed 16:30 A 053

MXenes as support for transition metal oxides electrocatalysts for water splitting application — •Axel Zuber[1], Zdeněk Sofer[2], and Michelle Browne[1] — [1]CE-NESD, Helmholtz Zentrum Berlin für Materialien und Energie, Berlin (Federal Republic of Germany) — [2]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague (Czeck Republic)

To reduce the cost of energy conversion and tend towards a greener energy production, research has been trying to use first-row transition metal-based catalysts for water splitting. Despite their good activity for the oxygen evolution reaction, transition metal oxides (TMOs) performance is hindered by their low conductivity and instability under potential. To improve it, recent works have successfully combined them chemically with conductive 2D transition metal carbides and nitrides (MXenes). The rich chemistry, large surface area and conductivity of MXenes make them excellent candidates as electrocatalyst supports, but they are also keen to oxidize in water which induces a loss of these properties. In this study, different MXenes were combined with transition metal oxides and tested as electrodes for the oxygen evolution reaction. The stability of the MXene structure as well as the resulting compound performance for the oxygen evolution reaction were investigated. The electrode materials remained stable and allowed to improve the oxygen evolution reaction overpotential of the transition metal oxide.

DS 9.6 Wed 16:45 A 053

Infrared and Raman spectroscopic analysis of functionalized graphene and Mxene layers — •Karsten Hinrichs[1], Mailis Lounasvuori[2], Fatima Akhtar[2], Namrata Sharma[2], Tristan Petit[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Application Laboratories Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH 14109 Berlin, Germany

Functionalized 2D-conductive materials like graphene and Mxene layers are interesting templates for catalysis but are also important for building of optical and electro-chemical sensors. Spectroscopic Raman and infrared (IR) ellipsometry analysis can access complementary information on the conductive material but also the ultrathin functional organic layer, respectively. Thereby bands due to molecular vibrations and phonons as well as free carrier absorptions are related to chemical and structural material properties. We acknowledge financial support by the European Union through EFRE 1.8/13.

DS 10: Thin Film Application

Time: Wednesday 15:00–18:15 Location: A 060

DS 10.1 Wed 15:00 A 060

Investigation of interfacial spin transport in chiral RhSi epitaxial thin films — •Surya Narayan Panda[1], Edouard Lesne[1], Qun Yang[1], Anastasios Markou[2], Binghai Yan[3], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]University of Ioannina, Greece — [3]Weizmann Institute of Science, Israel

The rise of nonmagnetic chiral topological semimetals as a uniquely attractive playground for the observation and control of various spin-orbit effects has ushered in the promising field of topological spintronics. In this work, we have investigated the spin-to-charge interconversion through spin pumping and inverse-spin Hall effect(ISHE) in sputter-grown epitaxial RhSi thin films and its subsequent transport across RhSi/Py interface. From the observed modulation of Gilbert damping parameter and ISHE voltage with RhSi thickness, the spin-Hall angle of RhSi and interfacial spin transparency of RhSi/Permalloy interface is determined. A stark variation of spin Hall angle and interfacial spin transparency is observed with ambient temperature in this heterostructure. The spin Hall angle and spin Hall conductivity is found to be maximum of 1.4% and 252 ($\hbar$/e) Ω^(-1) cm^(-1), respectively. A spin-mixing conductance and interfacial spin transparency as high as 34.7 nm-2 and 88% is attainable in these heterostructures. This study expands the horizon of topological spintronics and highlights the controlled spin-charge interconversion and interfacial spin-transport process in chiral semimetal/ferromagnet heterostructures.

DS 10.2 Wed 15:15 A 060

Functionalization of SiC diodes for soft X-ray optics — •Simone Finizio[1], Massimo Camarda[2], Joakim Reuteler[3], and Jörg Raabe[1] — [1]Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland — [2]SenSiC GmbH, Villigen PSI, Switzerland — [3]ScopeM, ETH Zürich, Zürich, Switzerland

Synchrotron light sources are a vital tool for the scientific community that has allowed for several critical discoveries. Amongst the quiver of techniques offered by synchrotrons, X-ray microscopy and spectroscopy are two of the most popular ones. A critical requirement for such techniques is the reliable and reproducible positioning of the X-ray beam, and the measurement of its intensity, to avoid measurement artefacts that can affect the quality of the acquired data. The integration of X-ray beam position and intensity sensors in measurement conditions as close as possible to those experienced by the sample under investigation is therefore of interest. In this presentation, we will show the fabrication and integration of SiC diode sensors with soft X-ray spectro-microscopy beamlines, in particular with geometries ranging from pinholes, center stops, and thin membrane films.

DS 10.3 Wed 15:30 A 060

Piezoelectricity enhances MoSe2 nanofowers adsorption of the antibacterial dye malachite green under sonication — •Jinzhu Wu — Harbin Institute of Technology, Harbin, China

Nanoscale piezoelectrics have recently found applications in radios, switches, tweezers, sensors, actuators, feld efect transistors and piezoelectric-gated diodes. Piezoelectrics may also be used to adsorb and efciently degrade pollutants, yet knowledge is actually scarce. Two-dimensional transition metal dichalcogenides were recently found to be piezoelectric. Here, MoSe2 nanofowers were synthesized by the hydrothermal method then used to adsorb the malachite green dye, an antifungal and antibacterial agent for aquaculture. Results show very high dye adsorption, of 85% within 5 s under sonication, with a theoretical maximum adsorption capacity of 208.3 mg/g.This is explained by spontaneous physisorption via pai-pai stacking interactions between aromatic malachite green and electron-rich MoSe2 nanofowers. For the frst time, this work clarifes that the piezoelectric efect of the few-layered MoSe2 nanofowers triggered by the ultrasonic vibration is a driven force for outstanding adsorption.

DS 10.4 Wed 15:45 A 060

Innovative Strategies in CZTS Solar Cells: Unravelling the Potential of Metal Substituted CZTS Thin Films — •Yusuf Selim Ocak[1,2], Ahmet Tombak[3], Mustafa Fatih Genisel[4], and Omer Celik[2,5] — [1]Institute of Nanotechnolgy, JUST, Jordan — [2]Smart-Lab, Dicle University, Turkey — [3]Department of Physics, Batman University, Turkey — [4]SESAME, Allan, Jordan — [5]LDMRC, University of Malaya, Malaysia

Copper zinc tin sulfide (CZTS) thin films are gaining traction in solar cell applications due to their abundance and favorable optoelectronic properties. This presentation provides a comprehensive exploration of CZTS thin films, focusing on strategically substituting metals to customize their optical, structural, and morphological traits.

We systematically examine the influence of metal substitutions like Si, Ge, Cd, and Ti on the structural properties and bandgap engineering of CZTS, shedding light on their potential as absorber materials. Additionally, we offer a detailed characterization of solar cells crafted from Cd- and Ti-substituted CZTS. The incorporation of various deposition techniques underscores the versatility of our approach, providing insights into how fabrication methods impact thin film properties.

This study enhances the fundamental understanding of CZTS thin films, emphasizing their practical significance in advancing solar cell technologies through tailored metal substitutions. The findings, supported by relevant literature, pave the way for the development of efficient and sustainable thin-film solar cells with enhanced performance characteristics.

DS 10.5 Wed 16:00 A 060

Tailoring gas permeation of carbon nanomembranes via the structure of molecular precursors — •Daniel Hüger[1], Anna-Laurine Gaus[2], Vladislav Stroganov[1], Julian Picker[1], Christof Neumann[1], Max von Delius[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Carbon nanomembranes (CNMs) are molecular nanosheets with a thickness of about 1 nm. They are synthesised via electron irradiation of aromatic self-assembled monolayers (SAMs), which enables to flexibly tailor their physical and chemical properties by choice of the molecular precursors. Among others, the permeation properties of CNMs make them promising for applications in energy storage and conversion. Here we present a study of the permeation of helium and water vapours through a series of CNMs synthesised from pyrene-1-thiol, anthracene-2-thiol, phenanthrene-2-thiol and 4'-nitro-4-biphenylthiol SAMs. We demonstrate that the introduction of functional groups on the CNM surface and tuning the precursors' structure significantly impact the permeation properties and therefore the selectivity of the permeating species.

DS 10.6 Wed 16:15 A 060

Reversible Photoalignment of Azobenzene inside the pores of thin MOF films — •Tillmann Koehler[1,2], Alexander Mundstock[3], Jürgen Caro[3], and Frank Marlow[1,2,4] — [1]Max-Planck-Institut für Kohlenforschung — [2]Universität Duisburg-Essen — [3]Leibniz Universität Hannover — [4]Center for Nanointegration Duisburg-Essen

Integrating molecular switches within the cavities of metal-organic frameworks (MOFs) represents a promising avenue for achieving all-optical switching - a crucial approach to address the escalating energy demands of contemporary internet and communication technologies. Our primary focus centers on employing azobenzene and its derivatives as guest molecules within these frameworks. Azobenzene can undergo photochemical switching between the stable trans-isomer and the metastable cis-isomer. As hosts, we utilize thin films of MOFs, a hybrid material class composed of metal centers interconnected by organic linkers. They are synthesized via liquid phase epitaxy by alternating exposition to metal and linker. The state of the isomers and their orientation inside the pores can be analyzed using linearly polarized UV/Vis spectroscopy. Our findings reveal that azobenzene encapsulated within the pores of MOF type HKUST-1 not only undergoes efficient isomerization, leading to reversible changes in optical properties, but also exhibits the uncommon phenomenon of photoalignment [1]. Results for higher loadings and more perfect films are shown. [1] J. Phys. Chem. Lett. 2021, 12, 36, 8903*8908

15 min. break

DS 10.7 Wed 16:45 A 060

Photosensitive silicon oxynitride doped silicon containing

wearable Bragg gratings against counterfeit applications — •Ali Karatutlu[1], Timuçin Emre Tabaru[1,2], Umut Taylan[1,3], Zehra Gizem Mutlay[1], Hamid-Reza Bahari[1], Esra Kendir Tekgül[1], Doğukan Hazar Özbey[1], Engin Durgun[1], and Bülend Ortaç[1] — [1]UNAM–Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, 06800-Turkey — [2]Sivas University of Science and Technology, Mecnun Otyakmaz Street No:1 Sivas 58100, Türkiye — [3]Empa, Swiss Federal Laboratories for Materials Science & Technology, Laboratory for Advanced Materials Processing, Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland

Bragg gratings are utilized in different advanced applications, including lasers, sensing, and spectrometers. This study demonstrates a synthesis of photo-sensitive silicon oxynitride-doped silicon containing distributed Bragg gratings (BGs) on a flexible substrate as a wearable material and utilization of this flexible material in the information storage inscribed by a femtosecond laser light. The BGs were designed and fabricated to possess a unique hyper-spectral reflection behavior from ultra-violet to near-infrared region. To make it user-friendly, the inscribed message *L* can be observed in an indoor or outdoor light at certain viewing angles, such as 45° with respect to the normal surface of the flexible BG. Furthermore, the message can also be observed at certain polarizations. Furthermore, we will show in the framework of ab initio calculations the first-time formation of silicon oxynitride crystals from Si3N4 crystals present in Si layers.

DS 10.8 Wed 17:00 A 060

Photoresponsive Nanoporous Metal Organic Framework Films with Switchable Unpaired Electron — •Yidong Liu and Lars Heinke — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Photoresponsive materials enable the dynamic remote control of their inherent properties. The integration of photochromic molecules within nanoporous metal organic frameworks (MOFs) offers a distinctive avenue for tailoring material attributes, including the interplay between the MOF host and guest molecules within the pores. In our study, a MOF film of HKUST-1 type with embedded hexaarylbiimidazole (HABI) photoswitches show reversible light-induced reactions between a stable HABI dimer state and a meta-stable radical state. The transitions between the dimeric and radical forms are characterized through infrared, UV-vis and electron paramagnetic resonance (EPR) spectroscopy. Through transient uptake experiments utilizing ethanol and methanol as probe molecules, we demonstrate that the dimer-radical switching profoundly influences the host-guest interaction, particularly altering the uptake amount and the diffusion rate of the guest molecules.

DS 10.9 Wed 17:15 A 060

Growth study of β-Ga_2O_3 on Ru(0001) substrates for resistive switching applications — •Aman Baunthiyal, Martin Williams, Alexander Karg, Marco Schowalter, Thorsten Mehrtens, Martin Eickhoff, Andreas Rosenauer, Jon-Olaf Krisponeit, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

β-Ga_2O_3 is in demand for high-power electronics, sensors, and UV devices. While Al_2O_3 and AlN are common substrates, this study aims for a metallic substrate serving as bottom electrode in vertically stacked resistive switching (RS) devices [1]. Here, we utilize Ru, which is also considered a promising replacement for Cu interconnects in CMOS technology due to its stable resistivity at high temperatures and excellent electromigration resistance.

After sputter deposition of Ru(0001) on Al_2O_3(0001) substrates at 450 °C, the subsequent growth of Ga_2O_3 was systematically studied with respect to growth temperature (room temperature to 600 °C) and film thickness. Raman spectroscopy unveiled that the growth of β-Ga_2O_3 growth starts at 200°C. Atomic force microscopy revealed an initial increase in roughness up to 400 °C and indicates a transition to a two-dimensional growth mode in the upper-temperature range. Finally, RS devices were created by deposition of Al top electrodes, featuring excellent stability with a consistent ON/OFF ratio exceeding $>10^4$ over extended retention and endurance cycles.

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

DS 10.10 Wed 17:30 A 060

Laser scanning induced phase transitions in V_2O_3 thin-films — •Stefan Guénon[1], Theodor Luibrand[1], Farnaz Tahouni-Bonab[1], Lorenzo Fratino[2], Amihai Kronman[3], Yoav Kalcheim[3,4], Marcelo Rozenberg[2], Ivan K. Schuller[4], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany — [2]Université Paris-Saclay, CNRS Laboratoire de Pysique des Solides, 9105, Orsay, France — [3]Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Technion City, 32000 Haifa, Israel — [4]Department of Physics and Center for Advanced Nanoscience, University of California - San Diego La Jolla, CA 92093, USA

There is a growing interest in strongly correlated insulator thin films in the emerging field of neuromorphic computing. Previous studies on the prototypical Mott-insulator V_2O_3 reported a strain induced spontaneous phase separation into metal-insulator herringbone domains during the Mott transition. Here, we used low-temperature optical microscopy to investigate the effect of laser scanning irradiation. We found that the response depends on the thermal history: When the film has been heated starting at a temperature below the Mott transition, the laser predominately induces a metallic phase. On the contrary, when the thin film has been cooled beginning at a temperature above the transition, the laser beam remarkably causes an insulating phase. Very likely this behavior is due to superheating and supercooling effects. Funding: Technion: ERC-2031938

DS 10.11 Wed 17:45 A 060

Non-volatile electro-thermal memristive behavior in planar $NdNiO_3$ thin film devices — •Farnaz Tahouni-Bonab[1], Matthias Hepting[2], Theodor Luibrand[1], Georg Cristiani[2], Gennady Logvenov[2], Bernhard Keimer[2], Dieter Koelle[1], Reinhold Kleiner[1], and Stefan Guénon[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Memristive two-terminal devices are heavily investigated in the emerging field of neuromorphic computing as building blocks for artificial neural network hardware, particularly for storing the synaptic weights via non-volatile resistive switching. Here, we report on a non-volatile electro-thermal memristive effect in a planar $NdNiO_3$ (7 nm thick) thin-film device due to its characteristic thermodynamic properties. This behavior was investigated by electrical transport measurement and simultaneous optical imaging. We found resistive switching via multiple persistent states, which can be directly related to the spatial geometry of the metallic shunt. These results can be understood by considering the electro-thermal instability caused by the resistance vs. temperature dependence.

DS 10.12 Wed 18:00 A 060

Developing neural networks for designing optical thin films — •Elena Stoyanova, Krassimir Panayotov, Tihomir Tenev, and Ilko Miloushev — Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee, Sofia 1784, Bulgaria

Almost every optical device is made up of a number of optical surfaces that guide and modify light as it passes through them. Optical coatings are produced as thin-film multilayers of different materials, using specialized deposition processes. Coatings are applied to optical components to guide and modify light as it passes through them and to use them at desired wavelength regions. Artificial Intelligence as neuron networks is included in the process of construction the thin films. Neural networks can learn and simulate complicated, nonlinear connections between input and output data. A computer program on Python is written, which investigates different layered structures in the spectral region between 0.2 *m and 2 *m. Film parameters values are given.

DS 11: Poster I (joint session DS/MM/O)

Time: Wednesday 17:00–19:00 Location: Poster B

DS 11.1 Wed 17:00 Poster B

Tailoring Ti3C2 MXenes towards the Oxygen Evolution Reaction — •Aline Alencar Emerenciano and Michelle Browne — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Ti3C2 MXenes are promising materials for water splitting due to their high conductivity, hydrophilicity, and good mechanical properties when compared to other 2D-nanomaterials [1]. The possibility of tailoring MXenes in terms of functional groups, flake size/shape, presence of defects, and surface area makes them excellent candidates to be hybridized with transition metal oxides. MXenes/TMO catalysts can provide synergetic properties such as high conductivity in combination with active sites for Oxygen Evolution Reaction (OER). To reduce the mass loading by increasing the intrinsic activity and stability of MXenes, the surface functionalization and surface area must be controlled. In this work, in situ generated HF was utilized to remove Al-elements for the production of Ti3C2. Synthesis protocols utilizing different concentrations of HCl were investigated to evaluate the flake quality in terms of functional groups distribution, flake size towards the existence of multilayered and delaminated nanoflakes, as well as the concentration of pin-roles on their surface. Overall, this work provides a better understanding in how HCl concentration can influence the MXenes contribution in hybrid electrocatalysts considering functional groups distribution and presence of defects.

1.Zhang, C. J. et al. Adv. Mater. 29, 1-9 (2017).

DS 11.2 Wed 17:00 Poster B

Chemical functionalisation of CuCo(2)-LDH on V(2)CT(x) for the oxygen evolution reaction — •Bastian Schmiedecke and Michelle Browne — Helmholtz-Zentrum Berlin, Berlin, Germany

MXenes, known for their exceptional surface area and high conductivity, serve as excellent catalyst supports, enhancing electrocatalytic performance in the oxygen evolution reaction (OER). Layered double hydroxide (LDH) materials, though promising for the OER, lack conductivity to ensure easy charge transfer during electrochemical processes. While, research on LDH materials has developed rapidly, there remains a high demand for refining the strategic combination of LDH with two dimensional (2D) materials, such as MXenes, which can significantly improve the water oxidation performance of LDH materials by inducing high conductivity, hydrophilicity and surface area.

This study introduces a hybrid catalyst, CuCo2-LDH grown on delaminated vanadium carbide (V(2)CT(x)) nanosheets to enhance the OER performance. The synthesized CuCo(2)-LDH@V(2)CT(x) electrocatalyst exhibited excellent activity with an overpotential of 289 mV at a catalytic current density of 10 mA cm-2 with a Tafel slope value of 74 mV dec-1. Furthermore, slight performance improvements were observed after 12 h of continuous operation. We propose that the enhanced performance is attributed to the conductivity of V(2)CT(x) and its synergistic interaction with CuCo(2)-LDH, effectively minimizing aggregation, exposing more active sites. This work demonstrates the significant potential of combining LDH-based nanomaterials with V(2)CT(x) MXene for energy conversion applications.

DS 11.3 Wed 17:00 Poster B

Analysis of polarization dependent IR spectra of thin films — •Karsten Hinrichs[1], Andreas Furchner[2], Fatima Akhtar[2], Norbert H. Nickel[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Application Laboratories Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH 14109 Berlin, Germany

The interpretation of bands in polarization dependent infrared (IR) spectra of thin films is addressed. Several examples such as an isotropic polymer film and functionalized silicon surfaces will be discussed as case studies. It will be shown that the observed vibrational band properties depend on the measurement geometry, the film thickness, the materials dielectric functions, as well as the direction of the probing electromagnetic fields. Comparative Density Functional Perturbation Theory (DPFT) - calculations are used for analysis. The financial support by the Europäischer Fonds für regionale Entwicklung by EFRE 1.8/13 and ProFIT 10185407 as well as the Federal Ministry of Education and Research and the project CatLab (03EW0015A/B) is acknowledged.

DS 11.4 Wed 17:00 Poster B

Focused-Ion-Beam induced Defect Emission in Hexagonal Boron Nitride — •Felix Schaumburg, Dominik Kaczmarek, David Plitt, Martin Geller, Günther Prinz, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Defects in the wide bandgap material hexagonal boron nitride (hBN) exhibit single-photon emission at room temperature (RT) [1]. We used the gallium ion beam of a focused ion beam (FIB) to generate ensembles of defects that we associated with boron vacancies having a photoluminescence emission exceeding 800 nm [2]. After irradiation isolated point defects can also be found next to the irradiated areas. We show that our created defects exhibit a bright RT emission, an almost sublinear power dependence commonly associated with a two-level system and an increasing signal, a decreasing full with at half maximum (FWHM), and a minimal shift to lower wavelengths at lower temperatures. Our results show, that we can generate bright emitters in hBN by Ga-ion treatment that are in a wavelength range of up to 800 nm. Our next goals will be contacting these emitters by putting a gate structure on top of it, as well as creating single defects at higher wavelengths. [1] F. Hayee et.al., Nat.Mater.19 (2020) [2] C. Qian et.al., arXiv (2022)

DS 11.5 Wed 17:00 Poster B

Optimizing electrical transport and SAW propagation in molybdenum disulfide — •Noah Spitzner[1], Pai Zhao[1], Renrong Liang[2], Chithra Sharma[1], Lars Tiemann[1], and Robert Blick[1] — [1]Center of Hybrid Nanostructures, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — [2]School of Integrated Circuits, Tsinghua University, 100083 Beijing, China

Few-layered and monolayer MoS_2 has gained increasing significance in recent years, due to its large band gap of up to 1.9 eV at the K and K′ valley of the hexagonal Brillouin zone. Surface acoustic waves (SAW) and transport measurements allow non destructive probing of the physics governing the material.

In this work we exfoliated MoS_2 flakes of a few layers onto a specially tailored substrate with $LiNbO_3$ as piezoelectric top layer. We can pass surface acoustic waves through the MoS_2 flake via an interdigitated transducer (IDT) electrode configuration and study the electrical response. To facilitate electron transport at low temperatures, liquid nitrogen physical vapor deposition (LNPVD) was utilized to deposit the contact metals. The cooled deposition reduces Fermi level pinning (FLP) in the contact interface and empowers us to measure longitudinal and transversal voltages with better contact quality.

Under acoustic excitation at 4.2 K, we observed acoustic currents and voltages in MoS_2 that depend on the power and frequency of the SAW. Hence, we were able to observe the acoustoelectric and acoustogalvanic effect. We also studied magnetotransport under perpendicular magnetic fields and the weak localization phenomenon.

DS 11.6 Wed 17:00 Poster B

Creating realistic carbon nanomembranes using molecular dynamics model simulations — •Levin Mihlan[1], Anna Niggas[2], Filip Vukovic[2], Jürgen Schnack[1], and Richard A. Wilhelm[2] — [1]Universität Bielefeld, Deutschland — [2]TU Wien, Österreich

1nm thin carbon nanomembranes (CNMs) are synthesized from aromatic self-assembled monolayers (SAMs) by electron-induced crosslinking and supposedly of irregular internal structure, which renders standard spectroscopic characterization very difficult [1]. However MD simulations can offer insights into CNMs' internal structure. Recently, it was shown that the neutralisation dynamics of highly charged ions (HCIs) transmitting through thin materials are very sensitive to the material structure [2]. Hence, HCI spectroscopy may, together with accompanying simulations using a time dependent potential [3], be used to characterize CNMs. In order to obtain model membranes whose mechanical and spectral properties , fit to those of manufactured CNMs, a model process starting from a SAM is implemented as an MD simulation. Structures generated this way can be compared to alternative model structures, which are created by incorporating experimental mechanical properties as input parameters. This approach

helps to gain a better understanding of the internal structure of CNMs.

[1] Dementyev et al. ChemPhysChem 21.10 1006 (2020)
[2] Wilhelm, Richard A. Surf.Sci.Rep. Vol 77 Issue 4 (2022)
[3] Wilhelm, Richard A; Grande, Pedro L.Commun.Phys.2,89 (2019)

DS 11.7 Wed 17:00 Poster B

Rolle of Collective Behavior of Water Molecules in Robust Ferroelectricity in Graphene Nanoribbons — •Igor Stanković[1], M. Awais Aslam[2], and Aleksandar Matković[2] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [2]Institute of Physics, Montanuniversität Leoben, Franz Josef Strasse 18, 8700 Leoben, Austria

An understanding of the water dynamics on the edges of one and two-dimensional structures is scarce. Still, such interactions can be sufficient to perturb local electric environments, therefore offering an opportunity to harness the effect of the local dipole moment of water. Combining experiments on nanoribbon field effect transistors and molecular dynamic simulations, we elucidate a collective behaviour of water within clusters adsorbed on graphene edges. We show that these nanoribbons exhibit significant and persistent remanent fields which can be employed in ferroelectric heterostructures and neuromorphic circuits.

References [1] M. A. Aslam et al, https://doi.org/10.48550 arXiv.2304.09738

DS 11.8 Wed 17:00 Poster B

Experimental setup for gas sensing with TMD based field-effect devices — •Axel Printschler[1], Emad Najafidehaghani[1], Antony George[1], Hamid Reza Rasouli[1], David Kaiser[1], Uwe Hübner[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena — [2]Leibniz Institute of Photonic Technology (IPHT), Jena

Sensing devices based on 2D transition metal dichalcogenides (TMDs) such as MoS_2, WS_2, $MoSe_2$, WSe_2, *etc.* have attracted significant research interest, as their electronic properties are greatly influenced by variations in the environment, *e.g.*, due to formation of adsorbates. This influence is reflected in changes of the device's electric transport characteristics, which can be precisely measured and used for gas sensing. As toxic gases pose a threat in many fields, there is a high demand in sensitive, selective and flexible gas sensors that also work at low power. Electronic sensors based on TMDs can satisfy this need while being atomically thin and flexible. Here we present an experimental setup and first results on gas sensing with field effect transistors (FETs) fabricated from TMD monolayers grown by chemical vapor deposition (CVD).

DS 11.9 Wed 17:00 Poster B

MOCVD synthesis of MoS2 and WS2 combination 2D heterostructures — •Nikolas Dominik, Sebastian Klenk, Florian Herdl, Cormac Ó Coileáin, Tanja Stimpel-Lindner, and Georg S. Duesberg — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, 85577 Neubiberg, Germany

Two-dimensional (2D) materials (such as MoS2 and WS2) are materials layered at the atomic scale. This gives them exceptional electrical, mechanical and optical properties, and makes them interesting for electronics, photovoltaics and sensing [1]. Van der Waals heterostructures composed of 2D materials expand on the possible range of properties and so have attracted extensive focus due to factors such as smooth heterostructure interfaces, ultrafast carrier transport, and high bandgap tunability [2].

Here we present the synthesis of MoS2/WS2 combination heterostructures via metal-organic chemical vapour deposition (MOCVD) using a high controllable industrial scale multi-precursor system, and show the clearly defined stacked nature of the films produced. We explore the growth parameter space using Raman and X-ray photoemission spectroscopy, and microscopy techniques. We complement our characterisation by examining the influences on the band structure of the layered material.

[1] Q. H. Wang et al., Nature Nanotech 7, 699-712 (2012)
[2] W. Xia et al., Nanoscale 9, 4324-4365 (2017)

DS 11.10 Wed 17:00 Poster B

RF-sputtering of Nb and NbN thin films for quantum transport studies — •Peer Heydolph, Vincent Strenzke, Isa Moch, Annika Weber, Lars Tiemann, and Robert Blick — Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Niobium plays a vital role in research and applications, contributing to advancements in superconductivity, quantum computing, and high-performance electronics. Here, we investigate the impact and interdependence of growth parameters on the properties of radio-frequency (RF)-sputtered niobium (Nb) and niobium nitride (NbN) thin films with a high critical temperature for applications in nanostructures and quantum transport studies at 4.2 Kelvin. We demonstrate that high quality superconducting films can be consistently produced even in a basic sputtering setup. We systematically varied the growth parameters such as the power of the RF-plasma and the flow of argon and nitrogen and survey their effects and interdependence on the properties of the thin films. The quality of the resulting films was characterized via X-ray diffraction (XRD), scanning electron microscopy (SEM) and profilometer measurements to gauge the film thickness. For electrical characterization at various temperatures and magnetic fields we employed a PPMS cryostat. We found that lower flow rates or RF powers do not necessarily lead to a higher critical temperature for NbN, which is in agreement with previous publications. Furthermore, it is crucial to finely tune all parameters and take into account their interdependencies.

DS 11.11 Wed 17:00 Poster B

Poly(neutral red) as a Possible Electrode Material for Electrochemical Cells — •Lisa Rohovsky[1], Daniel Holzhacker[1], Tsukasa Yoshida[2], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — [2]Department of Organic Materials Science, Graduate School of Organic Materials Science, Yamagata University

Poly(neutral red) (PNR) is used in sensors owing to its redox characteristics and high electrical conductivity. PNR is also easy to prepare and inexpensive. Therefore, it might also be of interest as an electrode material in electrochemical cells like, e.g., electrochromic cells, batteries, or dye-sensitized solar cells (DSSCs). In the latter case, it could even help to replace platinum as an electrode material, which is expensive and not readily available. In this study, thin films of PNR were prepared by an established electrosynthetic procedure by oxidation of neutral red by cyclic voltammetry (CV) in an aqueous solution.[1] Samples were produced for varied number of oxidative cycles and then analysed for their layer thickness and absorptance. As expected, the layer thickness increased linearly with the number of cycles, as did the absorptance. The reversible electrochemical reduction and reoxidation of aqueous solutions of ferro/ferricyanide in contact to the prepared films was studied as a model electrolyte. Results and implications for the applicability of such PNR electrodes will be discussed. [1]. Y. Harada, D. Kono, P. Stadler, T. Yoshida, SPAST Abstracts ,1(01), First International Conference on Technologies for Smart Green Connected Society 2021.

DS 11.12 Wed 17:00 Poster B

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

ScGaN can occur in various crystal orientations. The most important are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition can be found between these orientations. Plasma-assisted molecular beam epitaxy (PAMBE) in combination with reflective high-energy electron diffraction (RHEED) was performed to create layers with different scandium concentrations in ScGaN. To determine the concentration of the grown layers, X-ray photoelectron spectroscopy was used in the same vacuum chamber. In addition, the surfaces were analyzed using atomic force microscopy (AFM, in-situ) and scanning electron microscopy (SEM) to obtain information on the morphology of the surfaces and to confirm the gained crystal orientations X-ray diffraction (XRD) were performed.

DS 11.13 Wed 17:00 Poster B

Optical and morphological properties of thin Nb2O5 layers deposited via High Power Impulse Magnetron Sputtering — •Christof Zickenheiner[1], Raul Ramos[2], Viktor Udachin[1], Wolfgang Maus-Friedrichs[1], and José R.R. Bortoleto[2] — [1]Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [2]Instituto de Ciencia e Tecnologia, Sorocaba, Brazil

To address climate challenges and sustainable development, the UN

set ambitious goals. Renewable energy, particularly solar, plays a key role. Emerging technologies like perovskite solar cells (PSC) offer cost-effective production, competing with silicon-based counterparts. This study focuses on the electron transport layer in PSC using Nb_2O_5 thin films deposited on glass substrates via HiPIMS from an Nb-target in an Ar/O_2 atmosphere at 25 °C. Pulse duration and oxygen pressure were varied as experimental parameters. Optical emission spectroscopy (OES) revealed the presence of oxygen species within a plasma and excitation of sputtered metal species for the HiPIMS process. The examination of the morphological properties via profilometry and contact angle analysis showed an influence of the experimental parameters on roughness. That is, shorter pulses as well as lower oxygen pressure result in smoother layer growth with a lower deposition rate. The investigation of optical properties via UV/Vis-Spectroscopy showed no significant impact of pulse duration. It became evident that lower oxygen pressure reduces the incorporation of oxygen into the growing layer. This results in a changed phase composition, with the formation of NbO_2, which in turn affects optical and electrical properties.

DS 11.14 Wed 17:00 Poster B

An attempt to predict oligomer sputtering using binary collision approximation simulations — •Hans Hofsäss, Felix Junge, and Patrick Kirscht — II. Physikalisches Institut, Universität Göttingen, Germany

The binary collision approximation (BCA) program IMINTDYN [1] allows a prediction of ion solid interactions. For sputtering of carbon and SiO2 experimental sputter yields are significantly higher than yields from BCA simulations. SDTrimSP simulations [2] reproduce experimental sputter yields by adjusting the surface binding energies. For O atoms 1 eV instead of the elemental sublimation energy of 2.58 eV and for carbon 4.5 eV instead of 7.4 eV is used. For sputtering of carbon it was shown [3] that sputtering of oligomers and clusters is relevant. We introduce a model to simulate oligomer sputtering using the IMINTDYN program based solely on thermodynamic formation enthalpies. In particular sputtering of O2 and SiO dimers and carbon oligomers is energetically favorable. To predict the oligomer sputter fraction, we use Boltzmann factors based on the ratios of oligomer and monomer formation enthalpies. We show that we can quantitatively predict the carbon and SiO2 experimental sputter yields.

[1] H. Hofsäss, A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49

[2] A. Mutzke, R. Schneider, W. Eckstein, R. Dohmen, K. Schmid, U. von Toussaint, G. Bandelow, SDTrimSP Version 6.00, MPI Plasma Physics, report IPP 2019-02 (2019)

[3] E.Oyarzabal, R.P. Doerner, M. Shimada, G.R. Tynan, J. Appl. Phys. 104 (2008) 043304

DS 11.15 Wed 17:00 Poster B

Growth of Antimony thin films on c-plane Sapphire — •Jonathan Spelsberg, Alexander Fuhrich, and Martin Salinga — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Antimony has been demonstrated to function as a single-element phase change material for electronic memory applications [1]. Confinement into nanostructures is crucial for stabilizing the amorphous phase of this material that is otherwise known for its fast crystallization kinetics. Yet, the exact influence of interfacing dielectrics on the physical properties of Antimony requires a fundamental investigation. To this end, samples with a well-controlled interface are required. Here, we report about the growth of Antimony thin films on c-plane Sapphire by molecular beam epitaxy. Based on characterization with RHEED and AFM, we demonstrate the impact of substrate preparation and process temperatures on the growth of 3 nm to 30 nm thick antimony films. Moreover, we discuss the relevance of Antimony cluster size and the effective use of a cracker effusion cell.

[1] M.Salinga et al., Monatomic phase change memory, Nature Materials 17, p. 681-685 (2018)

DS 11.16 Wed 17:00 Poster B

Novel nanofabrication facility for ultra-clean samples — •Alexander Fuhrich and Martin Salinga — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the capabilities of a novel nanofabrication facility dedicated to the fabrication of nanostructures under ultra-clean conditions. In addition to a UHV cluster for MBE growth, the system comprises a lithography unit in an inert argon atmosphere. Air- and water-sensitive samples, like materials for memristive switches, can be structured using thermal scanning probe lithography with a lateral resolution down to less than 30 nm. Samples can be analyzed in-situ using RT-STM and RHEED. A self-sufficient UHV suitcase is used to characterize samples in other setups, such as femtosecond-laser pump probe spectroscopy, without ever exposing our samples to air.

DS 11.17 Wed 17:00 Poster B

Preparation and Characterization of Mixed Electrodes of WO_3 and MoO_3 as Electrochromic Coatings — •Smail Mekhilef, Thi Hai Quyen Nguyen, and Derck Schlettwein — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen

Electrochromic coatings can modify the transmittance for ambient light. As smart windows for buildings, relevant contributions can be expected for the energy-efficiency of buildings. Sputter- deposited WO_3 is typically used. Sustainability can be increased if low-temperature processes are established that would, further, allow the use of low-impact and low-weight polymer substrates. For large-scale applications, one may want to avoid W as a critical element and, at least partly, replace it by more abundant Mo. In this study, we extended established wet-chemical methods to prepare porous thin film electrodes of WO_3 [1] towards the processing of mixed oxides of W and Mo. Thin films of different W/Mo were prepared and characterized by scanning electron microscopy, atomic force microscopy and, mainly, by spectroelectrochemical measurements in contact to an inert organic electrolyte at either constant or swept electrode potential and the results will be discussed. [1]. T. H. Q. Nguyen, F. Eberheim, S. Göbel, P. Cop, M. Eckert, T. P. Schneider, L. Gümbel, B. M. Smarsly, D. Schlettwein, Enhancing the Spectroelectrochemical Performance of WO_3 Films by Use of Structure-Directing Agents during Film Growth, Appl. Sci. 2022, 12, 2327.

DS 11.18 Wed 17:00 Poster B

Deposition of reduced ceria thin films by reactive magnetron sputtering for the development of a resistive gas sensor — •Paul-G. Nitsch[1], Markus Ratzke[1], Emilia Pozarowska[2], Jan I. Flege[2], Carlos Alvarado Chavarin[3], Christian Wenger[3], and Inga A. Fischer[1] — [1]Experimentalphysik und funktionale Materialien, BTU-CS, Cottbus, Germany — [2]Angewandte Physik und Halbleiterspektroskopie, BTU-CS, Cottbus, Germany — [3]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The use of cerium oxide for hydrogen sensing is limited by the low electrical conductivity of layers deposited from a ceria target. To increase the electrical conductivity, partially reduced cerium oxide layers were obtained from a metallic cerium target by reactive magnetron sputtering. The proportions of the oxidation states Ce3+, present in reduced species, and Ce4+, present in fully oxidized species, were determined by ex-situ XPS. For electrical characterization, films were deposited on planarized tungsten finger electrodes. IV curves were measured over several days to investigate possible influences of oxygen and humidity on electrical conductivity. The morphological stability of the layers under ambient conditions was investigated by microscopical methods. The XPS results show a significant amount of Ce3+ in the layers. The electrical conductivity of as-grown samples is several orders of magnitude higher than that of samples grown from a ceria target. However, the conductivity decreases over time, indicating an oxidation of the layers. The surface morphology of the samples was found to be changing drastically within days, leading to partial delamination.

DS 11.19 Wed 17:00 Poster B

Modification of the optical and electrical properties of AZO thin films for variety of applications — •Maria Stefanova[1], Dimitrina Petrova[1,2], Blagovest Napoleonov[1], Stefani Bogoeva[1], Vladimira Videva[1,3], Velichka Strijkova[1], Vera Marinova[1], and Dimitre Dimitrov[1,4] — [1]Institute of Optical Materials and Technologies-BAS Sofia, Bulgaria — [2]South-West University "Neofit Rilski", Blagoevgrad, Bulgaria — [3]Sofia University, Sofia, Bulgaria — [4]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Here we report on the deposition of Aluminium Doped Zinc Oxide (AZO) thin films on sapphire substrates (AZO/Sapphire) by using ALD method and the influence of postdeposition UV-Ozone treatment on the films' properties. XRD revealed a polycrystalline wurtzite structure. The influence of UV-Ozone treatment on surface morphology, electrical and optical properties of AZO/Sapphire was investigated. It was found that UV-Ozone treatment improves the electrical and optical properties while did not cause significant changes to the polycrystalline structure and surface morphology of the AZO films which opens potential for various practical applications.

Acknowledgements This work is supported by the Bulgarian National Science Fund under the grant number KP-06-N-68/1 and the Research equipment of distributed research infrastructure INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science.

DS 11.20 Wed 17:00 Poster B

Transient Photoluminescence of Lead Halide Perovskites Beyond Lifetimes: Non-excitonic Geminate Pairs and Carrier Transport — •Hannes Hempel[1], Martin Stolterfoht[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin, Germany — [2]Chinese University of Hong Kong, China

Transient photoluminescence (trPL) is the standard technique to quantify the lifetimes of photogenerated charge carriers in energy conversion materials. However, trPL decays are sensitive to processes other than only carrier recombination. We show that the initial trPL transients of lead halide perovskite thin films on glass are dominated by charge transport, namely hot carrier transport, spread-out of non-excitonic gemmate pairs, and redistribution. Including these processes in the modeling of trPL yields the doping and intrinsic carrier concentration, the mobility and diffusion coefficient, the hot carrier transport length, and the radiative and non-radiative lifetimes. Further, we calibrate trPL to absolute photon numbers, which allows quantifying the transient quasi-Fermi-level splitting and reveals fundamental energy losses in photo absorbers such as the increase of entropy by loss of geminate correlation and redistribution. The presented analysis is crucial for the appropriate interpretation of trPL and yields almost all optoelectronic properties relevant for application as a photo-absorber in solar cells.

DS 11.21 Wed 17:00 Poster B

Ultrafast Lattice Dynamics in Epitaxially Grown Bismuth Thin Films — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], Abdur Rehman Jalil[3], Julian Mertens[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 epitaxially grown bismuth thin films on sub-ps timescales. Examination of reflectivity changes due to the coherent phonon response provides insight into the ultrafast lattice dynamics and relaxation of bismuth thin films. The pronounced thickness dependent behavior of bismuth is analysed by coherent phonons within the framework of displacive and impulsive excitation models. Here, we show how the competition of phonon softening due to different laser fluencies and phonon hardening from confinement effects can be understood. Raman measurements are carried out to help to disentangle both effects. XRD measurements are shown to help to understand the structural change of the lattice structure. These combined measurements will help to understand confinement and fluency effects in a single model and shows how to tune bonding properties in this unconventional class of materials.

DS 11.22 Wed 17:00 Poster B

Atomic-Scale Insights Into The Interlayer Characteristics of Thin-Layered Materials Using Ultra-high Vacuum Tip-Enhanced Raman Spectroscopy — •Soumyajit Rajak and Nan Jiang — University of Illinois Chicago, Chicago, USA

Optoelectronic properties of molecular thin films are controlled by the local nanostructures of a molecular arrangement. Probing the effect of the local environment of nanostructures is challenging because the spatial resolution of conventional optical spectroscopic techniques is limited by the diffraction limit of light. Coupling light with plasmonic nano-objects creates highly localized surface plasmons (LSPs), which allows us to break the diffraction limit. Herein we present a combined topographical and optical analysis of different surface-sensitive arrangements of molecules and 2D material heterostructures using angstrom-scale resolution scanning tunneling microscopy (STM) and ultra-high vacuum tip-enhanced Raman spectroscopy (UHV-TERS). TERS uses the apex of an STM tip made of a plasmonic metal to couple light to the near field. The Raman modes of the nanostructure underneath this tip are enhanced by the nano-confined surface plasmons which allows us to obtain chemical information with Angstrom scale spatial resolution. STM images combined with localized surface plasmon resonance-enhanced Raman signals reveal different adsorbate configurations of single molecule entities and a fundamental view of interfacial interactions. The atomic scale insights obtained into the local environment enable precise control over the fabrication of nanostructures with tailored optoelectronic properties.

DS 11.23 Wed 17:00 Poster B

In-situ Study of Surface Band-Bending in c-ZnO and its Effect on the Excitonic Dielectric Function — •Luis Rosillo Orozco[1], Kurt Hingerl[1], and Christoph Cobet[1,2] — [1]Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler Universität, Linz, Austria — [2]Linz School of Education, Johannes Kepler Universität, Linz, Austria

Semiconductors in air and in vacuum often have a band-bending near the surface caused by surface states capturing bulk charges or simply due to natural polarization in the case of polar materials, as is the case of Zinc Oxide. Nevertheless, when semiconductors are in contact with an electrolyte we can intentionally produce a surface dipole and create a space charge region (SCR) by adding another electrode in the solution and applying a voltage between the two.

Space charge regions have a big impact on the optical and electrical properties of semiconductors and, of course, semiconductor devices. Therefore, it is of high interest to understand the effects caused by them.

We present in-situ spectroscopic ellipsometry (SE) combined with electrochemical techniques to study the response of the discrete excitons and exciton-phonon complexes (EPC) to the inner electric fields produced near the semiconductor surface. Using mono-chromatic transients we are able to identify the flat-band potential. A semi-empirical optical model is developed to study the contribution of the surface band-bending to the total dielectic function for a range between 3.2 e.V. to 3.6 e.V.

DS 11.24 Wed 17:00 Poster B

In situ optical tracking of oxidation state changes of NiFe alloys by Reflectance Anisotropy Spectroscopy — •Sandhya Chandola[1], Karuppasamy Dharmaraj[2], Jörg Rappich[1], Norbert Esser[3,4], and Sonya Calnan[2] — [1]Young Investigator Group Nanoscale Solid-Liquid Interfaces (CE-NSLI), Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Kompetenzzentrum Photovoltaik Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [4]Leibniz-Institut für Analytische Wissenschaften ISAS e.V., Schwarzschildstr. 8, 12489 Berlin, Germany

The oxygen evolution reaction (OER) is a key reaction involved in water splitting and has attracted increasing attention for hydrogen generation for clean energy uses. Nickel/iron (NiFe)-based compounds have been known as active OER catalysts for decades, and there has been increasing interest in developing NiFe-based materials for higher activity and stability.

Reflection Anisotropy Spectroscopy (RAS) in the visible spectral range is a polarisation sensitive optical spectroscopy technique used to study morphological and electronic structure changes of surfaces and thin films in-situ. It achieves high sensitivities in the detection of ultrathin layer structures down to the sub-nanometer scale and can follow the optical changes of the surface during catalytic reactions. By combining in-situ RAS and cyclic voltammetry (CV), the changes in both the redox state and structural phase during OER activity of NiFe alloys can be optically tracked.

DS 11.25 Wed 17:00 Poster B

Triptycene as a versatile building block for self-assembled monolayers — Takanori Fukushima[1], Manfred Buck[2], Egbert Zojer[3], and •Michael Zharnikov[4] — [1]Tokyo Institute of Technology, Yokohama 226-8503, Japan — [2]EaStCHEM School of Chemistry, University of St Andrews, St Andrews KY16 9ST, UK — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria — [4]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

When employing self-assembled monolayers (SAMs) for tuning surface- and interface-properties, a strong binding to the substrate, structural uniformity, and the ability to align functional groups and to control their density are desirable. To achieve these goals, tripod systems bearing multiple bonding sites have been developed as an alternative to conventional monodentate systems. A bonding of all three sites has, however, hardly been achieved with the consequence that structural uniformity and orientational order in tripodal SAMs are usually quite poor. To resolve that problem, we designed a series of triptycene-based molecules decorated with three anchoring groups, which can be assembled on different substrates. Depending on the character of the anchoring groups, well-defined tripodal SAMs could be prepared

on Au(111), Ag(111), and indium tin oxide. Either unsubstituted or differently substituted triptycene-based molecules were assembled in context of different issues, viz. (i) homogeneous tripodal assembly, (ii) polymorphism and hidden chirality, (iii) on-surface click chemistry, (iv) multiple pathways in charge transfer, and (v) nanofabrication.

DS 11.26 Wed 17:00 Poster B

A new design concept for SAMs of N-heterocyclic carbenes — Mateusz Wróbel[1], Daria M. Cegiełka[1], Andika Asyuda[2], Krzysztof Kozieł[3], •Michael Zharnikov[2], and Piotr Cyganik[1] — [1]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [3]Faculty of Chemistry, Jagiellonian University, 30-387 Krakow, Poland

Self-assembled monolayers (SAMs) of N-heterocyclic carbenes (NHCs) on metal substrates are currently one of the most promising systems in context of molecular engineering of surfaces and interfaces. Interest in these systems is mainly driven by their assumingly higher thermal stability compared to thiolate SAMs most broadly used at the moment. Most of the NHC SAMs utilize imidazolium as an anchoring group for linking molecules to the metal substrate via carbene C atom. It is well established in the literature that upright-oriented and stable NHC SAMs can only be built when using bulky side groups attached to nitrogen heteroatoms in imidazolium moiety, which, however, reduce significantly the packing density. In contrast, combining several complementary experimental techniques, we show that aromatic monolayers exhibiting at least double surface density, upright molecular orientation, and ultra-high thermal stability compared to the NHC SAMs reported before can be readily fabricated on the basis of NHCs with small methyl side groups in combination with simple solution-based preparation procedure. These parameters are crucial for numerous applications, including molecular and organic electronics.

DS 11.27 Wed 17:00 Poster B

Interaction study between thin films of polyvinyl acetate and (plasma-treated) aluminum — •Sascha Zimmermann[1], Philipp Moritz[1], Oliver Höfft[1], Lienhard Wegewitz[1], Wolfgang Maus-Friedrichs[1], and Sebastian Dahle[2] — [1]Clausthal University of Technology, Germany — [2]University of Ljubljana, Slovenia

Composite materials made of wood and aluminum are becoming increasingly popular due to the combination of their properties. However, in order to exploit these advantages, the two materials must be bonded with sufficient stability. While the adhesive polyvinyl acetate (PVAc) exhibits high adhesive strength on wood, its bonding capabilities with aluminum are limited. The surface of the aluminum must therefore be modified. In this work, the aluminum surface is treated with a dielectric barrier discharge plasma in air with the aim of enabling molecular interactions. Various analytical techniques, including X-ray photoelectron spectroscopy (XPS), Reflection Absorption Infra-Red Spectroscopy (RAIRS) and Atomic Force Microscopy (AFM), are employed to analyse the chemical interactions between aluminum and PVAc. This involves producing nm-thin films using spin coating. For untreated aluminum, no interactions were detected. AFM revealed the inability to deposit nanometer-thin films due to the lack of interactions, leading to the formation of PVAC-clusters. Plasma-treated aluminum led to a stronger chemical shift in the XPS spectra indicating hydrogen bonding. This finding was confirmed by RAIRS, which shows bands associated with hydrogen bonding.

DS 11.28 Wed 17:00 Poster B

Spectroscopical properties investigation of pyrene based molecules in perspective of singlet fission — •Sruthy Asa Rajan, Sergey Bagnich, and Anna Köhler — Universität Bayreuth, Bayreuth, Germany

Photovoltaics plays a vital role in renewable energy. Theoretically, convectional silicon solar cells' efficiency is limited to 33% known as the Shockley-Queisser limit, which is limited by some practical and fundamental losses like thermalisation loss. Singlet fission (SF) is a carrier multiplication process, which has the potential to overcome Shockley-Queisser limit. In an organic semiconductor, chromophore in its singlet excited state shares its energy with a nearby ground-state chromophore to form two triplet excitons. Recent studies shown that some pyrene derivatives exhibit SF. A study has shown that bridged SF chromophore forms generated triplet pair and hence leading to formation of long-lived triplets.

We are investigating the impact on absorption, photo-luminescence, lifetime decay, time-resolved spectroscopy and quantum yield of different N-substitution groups on para Diketopyrrollopyrrole (PDPP) based pyrene derivatives, which have a comparable triplet energy to silicon bandgap. We will focus more on the changes in morphology of film of these compounds by varying the conditions of film preparation, such solvents, annealing effect, etc. We hypothesis that certain orientation of these pyrene-base molecules can trigger singlet fission.

DS 11.29 Wed 17:00 Poster B

Understanding the disparate interactions of thin polymer films with natively oxidized metal surfaces and metal oxide crystals — •Friedrich Bürger, Philipp Moritz, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

In the Collaborative Research Centre 1368 "oxygen free production" the molecular interactions between thin films of commonly used polymers, poly(ethyl cyanoacrylate) (PECA) and poly(methyl methacrylate) (PMMA), and different metal oxides have been characterized. In the context of this project, certain interactions became apparent, e. g. hydrogen bonding or ionic interactions that were observed on natively oxidized samples representing very thin oxide films. In contrast, these interactions were absent on a TiO_2 single crystal. To investigate if this effect is reproducible and inherent to metal oxide single crystals, the interactions of PECA and different metal oxide single crystals are determined using X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS) and Metastable Induced Electron Spectroscopy (MIES). These results are compared to the interactions of natively oxidized metal samples with thin polymer films. Assuming reproducibility, a root cause for the disparate interactions is proposed.

DS 11.30 Wed 17:00 Poster B

Influence of processing atmospheres on curing and bonding of cyanoacrylate adhesives — •Philipp Moritz, Oliver Höfft, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Technical University Clausthal, Clausthal-Zellerfeld, Germany

Cyanoacrylates are fast-curing adhesives that are often used in joining technology to bond components together quickly. The curing and strength of the bond are often improved with numerous additives and surface pre-treatments. However, the surrounding process atmosphere is an aspect that has hardly been used to control curing and adhesive interactions.

To investigate the interactions and curing, thin films of cyanoacrylate are deposited on natively oxidized copper substrates. The surrounding atmosphere is varied between (i) air atmosphere, (ii) argon and (iii) an oxygen-free environment (O_2 partial pressure $< 10^{-20}$ mbar). The curing and underlying molecular interactions at the interface between cyanoacrylate and oxidized copper are investigated using spectroscopic and microscopic methods.

Curing in argon and the O_2-free atmosphere is significantly slower than in air. Nevertheless, strong interactions occur in an oxygen-free atmosphere and air, e.g. hydrogen bonds and ionic interactions. In argon, on the other hand, no molecular interactions are observed.

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DS 11.31 Wed 17:00 Poster B

The influence of PDMS residues on the mobility of molecules deposited onto Si/SiO2 wafers — •Erik von der Oelsnitz[1,2], Tim Völzer[1,2], Julian Schröer[1], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institute of Physics, University of Rostock, Germany — [2]Department "Life, Light & Matter", University of Rostock, Germany

The exfoliation and stamping of flakes of 2D materials onto a substrate is one of the most used methods for the preparation of transition metal dichalcogenide (TMDC) monolayers. However, it was found that during the transfer of the flake, impurities and in particular residues of the common stamp material polydimethyl siloxane (PDMS) are transferred to the substrate. This could have a major impact when analyzing TMDCs, especially in TMDC/molecule hybrid structures. In order to examine the effect of these impurities, dye molecules were evaporated onto a Si/SiO2 wafer and then measured in a fluorescence lifetime microscope (FLIM). Here, in a certain area, the dye coverage is removed by laser-induced photodegradation and the diffusion of the molecules into this depleted area is examined. Three wafers are compared, each representing a specific step of the preparation process. The FLIM measurements showed that the molecules on the bare wafer

diffuse into the depleted area the fastest, while they take significantly longer on the samples that came into contact with PDMS. This shows that the surface properties of exfoliated 2D materials are significantly influenced by the contact with PDMS, which in turn has a major effect on the mobility and thus the dynamics of deposited molecules.

DS 12: Hertha Spohner Prize Talk

Time: Wednesday 17:30–18:00 Location: A 053

Prize Talk DS 12.1 Wed 17:30 A 053

Metal Halide Perovskites - Tuning the Next Generation of Solar Cells — •Juliane Borchert — University of Freiburg INATECH Solar Info Center, Emmy-Noether-Straße 2, 79110 Freiburg im Breisgau, Germany — Fraunhofer ISE Heidenhofstr. 2, 79110 Freiburg im Breisgau, Germany — Laureate of the Hertha-Sponer-Prize 2024

The looming climate crisis makes a rapid transition towards renewable energies necessary. One major contributor to this transition are photovoltaic solar cells. They enable us to harness the energy of the sun. Currently the vast majority of commercially available solar cells are based on the semiconductor silicon. In the last decades a lot of research and development has gone into the optimization of silicon solar cells. As a result, their efficiencies are now coming close to the theoretical limit for silicon and new strategies and materials are needed to further improve solar cells. A very promising group of materials are the metal halide perovskites. They combine many intriguing properties from a tunable bandgap to processibility at low temperatures. This has led to them being investigated for use in a wide range of semiconductor devices including solar cells and LEDs as well as photodetectors, transistors and even lasers. In this talk I will introduce you to this intriguing material class and show promising methods to scale it to industrial sizes. I will give insights into the advantages of vacuum-based deposition techniques and the high solar cell efficiencies that have been achieved with them. I will also illuminate which gaps in understanding need to be investigated further and how this research area may develop in the coming years.

DS 13: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides II (joint session DS/MM/O)

Surface functionalization & defects and Water & gas Interaction

Time: Thursday 9:30–12:15 Location: A 053

Invited Talk DS 13.1 Thu 9:30 A 053

Computational insights into the surface functionalization and defects in MXenes — •Hannu-Pekka Komsa — Microelectronics Research Unit, University of Oulu, Finland

Two-dimensional (2D) transition metal carbide and nitride MXenes offer rich chemistry with extraordinary properties. The surface of MXenes is terminated by -O, -OH, and -F groups during the synthesis. However, there is limited understanding on how the surface composition depends on the synthesis conditions and on the type of MXene (transition metal, carbon vs. nitrogen, and the number of atomic layers).

We developed a multi-scale computational scheme to simulate the distribution and the thermodynamically favorable composition of the functional groups on the MXene surfaces. We considered the most popular MXene systems such as Ti_2C, Ti_3C_2, Ti_2N, Ti_4N_3, Nb_2C, and Nb_4C_3. The surface accommodates mixtures of functional groups for all considered MXenes with similar distributions regardless of the type of metal, carbon or nitrogen species and number of atomic layers. These findings are shown to be important for an accurate prediction of properties and stability of these materials. Next, we investigated the propensity of metal vacancy formation under synthesis conditions. The results suggest that vacancy formation is crucial step in initiating MXene oxidation. Finally, to support experimental characterization, we simulated the Raman spectra as a function of functional group distribution, temperature, and disorder, and the materials' response to electron irradiation in electron microscope.

DS 13.2 Thu 10:00 A 053

In situ monitoring of surface termination of Ti3C2Tx MXene with Raman spectroscopy — •Julian Plaickner[1,2], Tristan Petit[2], Peer Bärmann[2], Thorsten Schultz[2,3], Norbert Koch[2,3], and Norbert Esser[1,4] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstrasse 36, 10623 Berlin — [2]Hardenbergstrasse 36 — [3]Institut für Physik & IRIS Adlershof, Humboldt Universität zu Berlin, 12489 Berlin — [4]Leibniz Institut für Analytische Wissenschaften ISAS eV, Schwarzschildstrasse 8, 12489 Berlin

In the last years, MXenes have attracted attention due to an interesting combination of physical properties. A better knowledge of the surface chemistry of MXenes is critical for the implementation in applications. A promising investigation approach is annealing-induced desorption of surface terminations, because it might make the surface very active for further functionalizations. In this work, the effect of annealing on the Ti3C2Tx MXene surface chemistry in UHV has been investigated with Raman spectroscopy in ultra-high vacuum. Changes in the Raman spectra are correlated with the desorption of the major part of the F surface termination at 650 °C. Most of the observed spectral features show a significant broadening already before annealing. We attribute this to the intrinsic disordered nature of the MXenes due to a mixed surface termination and a broad background associated to electronic Raman scattering. With this study we identified of the vibrational signatures associated with F-termination and provided new insights into the interpretation of the vibrational spectra of Ti3C2Tx MXenes.

DS 13.3 Thu 10:15 A 053

Hydrogenation as a mean to remove halogen functionalization from of Ti3C2Tz thin films — •Silvano Lizzit[1], Florian Brette[2,3], Hanna Pazniak[4], Monika Shied[1], Paolo Lacovig[1], Florent Boucher[3], Vincent Mauchamp[2], and Rosanna Larciprete[5] — [1]Elettra-Sincrotrone Trieste, Trieste (I) — [2]Uni. Poitiers, ISAE-ENSMA, CNRS, PPRIME, Poitiers (F) — [3]CNRS-IMN, Nantes (F) — [4]Uni. Grenoble Alpes, CNRS, Grenoble INP, Grenoble (F) — [5]CNR- ISC, Roma (I)

The nature and the density of the chemical groups terminating the MXenes surface determine their electronic and chemical properties. Therefore, the manipulation of the surface termination allows to change the way these compounds interact with the surrounding environment. In this study we explored the possibility of using the functionalization with H atoms as a mean to modify the surface termination of T3C2Tz thin films. To this aim we used photoelectron spectroscopy with synchrotron radiation to investigate the surface reactions induced by the exposure to atomic hydrogen. Simulation of the valence band spectra by DFT calculations combined with the analysis of the core level spectra allowed us to elucidate the changes in the chemical bonding determined by the interaction with H atoms. It turned out that, in addition to the formation of C-H and -O-H bonds, sample hydrogenation removed the halogen terminating atoms, decreasing the F and Cl concentrations to less than 20% of the initial values. After removing the hydrogenated phases at 400 K, the dehydrogenated surface exhibited a chemical reactivity higher than that of the pristine sample.

DS 13.4 Thu 10:30 A 053

Chemical characterization of defects in Ti3C2Tx MXenes by soft X-ray spectroscopy — •Arsène Chemin[1], Zoé Dessoliers[1], Robert W. Lord[2], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]A.J. Drexel Nanomaterials Institute, Drexel Uni-

versity, Philadelphia, Pennsylvania, USA

MXenes offer a wide spectrum of properties with numerous fields of application. Yet, these properties can be strongly affected by defects, and a detailed understanding of their nature and structure is essential. Despite many observations of such defects, grasping their chemical natures is challenging. In this work, high-resolution X-ray Photoelectron Spectroscopy (HR-XPS) and, at the Ti L- and C,O K-edges, soft X-ray Absorption Spectroscopy (XAS), performed at the BESSY II synchrotron in Berlin, are used to investigate the chemical nature of defects in Ti3C2Tx MXenes.

15 min. break

Invited Talk DS 13.5 Thu 11:00 A 053

MXenes as materials for carbon capture, storage, and usage technologies: Computational insights & predictions — •Francesc Viñes — Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1-11, 08028 Barcelona, Spain

Environmentally-wise, pristine MXenes have been proposed as suited materials for carbon capture and storage (CCS) technologies, as predicted by computational density functional theory (DFT) simulations on suited models.1 Such MXenes display a high affinity towards carbon dioxide (CO2), strongly binding it, and activating it by charge transfer, gaining a bent CO2 with elongated bonds. The CCS capabilities highlighted through kinetic phase diagrams (KPD) were confirmed by experiments,2 showing a high CO2 uptake due to the MXene high surface area, specially high when MXene is made of light transition Ti or V metals. Furthermore, given the CO2 activation pristine MXenes can be used in carbon capture and use (CCU) technologies, acting as heterogeneous catalysts. A recent DFT study shows MXenes use as heterogeneous catalysts for the reverse water gas shift reaction (RWGS), where a KPD analysis reveals a swing mode RWGS operation, where CO2 is first converted into CO oxidizing the MXene surface, later regenerated by hydrogen treatment releasing water.

1 Morales-García et al. J. Mater. Chem. A 6 (2018) 3381. 2 Persson et al. Adv. Mater. 31 (2019) 1805472. 3 Morales-Salvador et al. ACS Catal. 11 (2021) 11248.

DS 13.6 Thu 11:30 A 053

Effect of Surface Terminations on the Water Intercalation into Ti3C2Tz MXene Thin Films — Aditya Sharma[1], Thierry Ouisse[1], Ulf Wiedwald[2], Andrei Chumakov[3], Fabrice Wilhelm[4], and •Hanna Pazniak[1] — [1]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France — [2]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Duisburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

MXenes are 2D materials whose surface is terminated by functional groups that drastically affect the properties of MXenes, including their affinity for water. In this study, we synthesized Ti3C2 MXenes with 1) mixed (=O, -F, and -OH) and 2) halogen (-Cl) terminations and prepared thin films by drop casting. X-ray absorption near edge structure shows different local chemical environment of Ti depending on the terminations, which is also confirmed by density functional theory. Next, we expose the MXene thin films to various humidity levels and studied the water intercalation by wide angle X-ray scattering. We observed that the interplanar spacing of mixed-terminated MXenes varied from 11.74 Å to 16.97 Å with increasing relative humidity from 0% to 100%, respectively. In the Cl-terminated MXenes, however, the interplanar spacing remains much smaller and only changes from 11.0 Å to 12.8 Å as function of relative humidity. In both cases, the process of water intercalation is reversible.

Funded by ANR-23-CE09-0031-01 project.

DS 13.7 Thu 11:45 A 053

Isotopic Analysis of Intercalated Protons in $Ti_3C_2T_x$ MXene for Electrochemical Energy Storage using in-situ FTIR Spectroscopy — •Andreas Weisser[1], Mailis Lounasvuori[1], Namrata Sharma[1], Kyle Matthews[2], Teng Zhang[2], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [2]A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

MXenes, a family of 2-dimensional transition metal carbides, are a promising candidate for use in energy storage applications due to their high capacitance. Here, we monitor the confined water and protons in $Ti_3C_2T_x$ MXene electrodes during cyclic voltammetry using operando FTIR spectroscopy. Isotopic exchange with deuterium oxide is used to allow for a better understanding of the proton dynamics inside the MXene interlayers. In-situ FTIR measurements are being performed with a dedicated electrochemical cell able to measure the different vibrational modes of the confined species. The measurements are conducted in attenuated total reflectance mode (ATR).

The focus of this presentation will be on analyzing the change of the vibrational modes of water and deuterium during electrochemical cycling versus the applied potential to the working electrode. This behaviour will be discussed with regard to the intercalation of protons and the reordering of the intercalated water or deuterium. The results will be placed in the context of MXene in the role of an electrode for pseudocapacitor applications.

DS 13.8 Thu 12:00 A 053

Electronic Structure of V2CTx MXene in aqueous solutions studied using in situ Scanning Transmission X-Ray Microscopy. — •Namrata Sharma[1], Kyle Matthews[2], Andreas Weisser[1], Mailis Lounasvuori[1], Markus Weigand[1], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie GmbH, 12489 Berlin, Germany — [2]A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering Drexel University Philadelphia, 19104 PA, USA

MXenes, a class of 2D transition metal carbides and nitrides have attracted much attention in many applications, thanks to their layered structure, hydrophilicity, and surface terminations. Recently, a new synthesis protocol has significantly improved the quality and shelf life of V2CTx MXene. This study focuses on the behaviour of V2CTx MXene in aqueous solutions studied using In-situ Scanning Transmission X-Ray Microscopy (STXM) with dedicated electrochemical flow cell at the synchrotron BESSY II. STXM provides element-specific nanomaterial electronic structure characterization in liquid at ~50nm spatial resolution. Here we characterize the electronic structure of pristine and aged V2CTx MXene in air, water, ZnSO4, and H2SO4, using X-ray Absorption Spectroscopy (XAS) at V L-edge and O K edge. The stability of individual V2CTx MXene flakes is monitored through high resolution chemical imaging over several hours in aqueous electrolyte. In this work we stress upon on the relevance of chemical imaging allowed by STXM for insights into oxidation and hydrolysis of MXene in aqueous environment at the nanoscale.

DS 14: Transport Properties

Time: Thursday 9:30–10:15 Location: A 060

DS 14.1 Thu 9:30 A 060

Influence of the microstructure on the impedance of microstructured ceria thin films — •Jan L. Dornseifer[1,2], Janis K. Eckhardt[2,3], Mattias T. Elm[1,2,3], 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 — [3]Institute of Physical Chemistry, Justus-Liebig-University, Giessen, Germany

Polycrystalline thin films with mixed electronic and ionic conductive properties are essential for many energy devices. Their charge transport properties are often characterized by impedance spectroscopy (IS). The IS data is usually evaluated by using simple circuit models to correlate macroscopic properties with microscopic transport processes. Here, we show that the microstructure in polycrystalline ceria thin films has a significant impact on the impedance. An experimental approach has been developed to prepare ceria microstructures on sapphire substrates. Utilizing a lithographic process, single ceria microstructures were electrically contacted and investigated by IS. Novel computer-aided simulations based on an impedance network model are used to analyze the experimental IS data. In these simulations, the real ceria microstructure is accurately mapped and implemented. The results show that the influence of the microstructure on the impedance is stronger than previously thought. Further investigations are promising for establishing a new correlation model.

DS 14.2 Thu 9:45 A 060

Magneto-transport characterization of ultra-thin corrugated Cr2O3/Co/Pt layers — •Shahrukh Shakeel, Oleksandr Pylypovskyi, Pavlo Makushko, Denise Erb, Shengqiang Zhou, René Hübner, Jose Angel Fernandez Roldan, Olha Bezsmertna, Jürgen Fassbender, Oleksii Volkov, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e. V., Dresden, Germany

Chiral magnetic textures are formed in low-dimensional ultra-thin magnetic systems due to the presence of intrinsic Dzyaloshinskii-Moriya interaction (iDMI), appearing due to the breaking or lack of inversion symmetry at the film interfaces [1]. Alternatively, in curvilinear magnetic systems, exchange-induced or extrinsic DMI (eDMI) emerges due to the geometrical breaking of local inversion symmetry [1]. The synergy between iDMI and eDMI, resulting into a mesoscale value of DMI (mDMI), enables the tunability of magnetochirality by selecting application specific material and geometry [1]. We studied this interplay by magneto-transport measurements of ultra-thin corrugated Cr2O3/Co/Pt layers with perpendicular magnetic anisotropy to calculate the effective spin-orbit torque (SOT) fields [4] and subsequently the mDMI strength for flat (reference) and corrugated samples. Whereby, a change in mDMI strength is observed due to the corrugations. Furthermore, the angular dependence of mDMI with respect to the angle between the crosses and corrugations was explored. References [1] O. Volkov et al., Sci. Rep. 8, 866 (2018). [2] J. Kim et al., Nat. Mat. 12, 240-5 (2012).

DS 14.3 Thu 10:00 A 060

Magneto transport in bilayer graphene cavities — •Florian Schöppl, Michael Barth, Klaus Richter, and Angelika Knothe — Institut für Theoretische Physik, 93053 Regensburg, Germany

The remarkable sample quality of bilayer graphene in combination with the unprecedented electronic control of the band-structure makes bilayer graphene an excellent platform for electron optics. While the purity of the system allows for ballistic transport on the micrometer scales [1,2], the trigonal warping of the band structure close to each K points induces a valley dependent selection of momenta leading to unique transport and scattering properties [3,4]. Interested in the interplay of symmetry breaking induced by a variety of all-electronic gate confinements and the trigonal warping, we implement various quantum mechanical tight binding models and deploy them to investigate magneto transport through bilayer graphene cavities.

[1]L. Seemann A. Knothe M. Hentschel, Gate-tunable regular and chaotic electron dynamics in ballistic bilayer graphene cavities, Phys. Rev. B (2023) [2]L. Banszerus M. Schmitz S. Engels M.Goldsche K. Watanabe T. Taniguchi B. Beschoten Ch. Stampfer, Ballistic Transport Exceeding 28μm in CVD Grown Graphene, Nano Lett. 2016 [3]C. Gold A. Knothe A. Kurzmann A. Garcia-Ruiz K. Watanabe T. Taniguchi V. Fal*ko K. Ensslin T. Ihn, Coherent Jetting behind a gate-defined channel in bilayer graphene, Phys.Rev. Lett. (2021) [4]J.K. Schrepfer S.C. Chen M.H. Liu K. Richter M. Hentschel, Dirac fermion optics and directed emession from single- and bilayer graphene cavities, Phys. Rev. B (2021)

DS 15: Thermoelectric and Phase Change Materials

Time: Thursday 10:30–12:00 Location: A 060

DS 15.1 Thu 10:30 A 060

Force constants and bond strength in elemental electron rich Sb — •Franziska Zahn[1], Christopher Benndorf[2], Hans H. Falk[1], Konrad Ritter[1], Eva M. Zollner[1], Sergiu Levcenko[1], Edmund Welter[3], Oliver Oeckler[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Mineralogy, Crystallography and Materials Science, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The valence-electron count of the group V metalloid Sb is 5, corresponding to an electron rich system similar to many thermoelectric and phase change materials such as GeTe and PbTe. Elemental Sb exhibits a layered structure, where each Sb atom has three short and three slightly longer first neighbor bonds. To study the structural and vibrational properties of Sb in more detail, extended X-ray absorption fine structure spectroscopy (EXAFS) was performed at the Sb K-edge at ten different temperatures ranging from 20 K to 295 K. The temperature dependence of the bond length variation σ^2 (mean square relative displacement) was evaluated using a correlated Einstein model, providing static disorder and bond-stretching force constants. Interestingly, the force constant of the long first neighbor bond is ~ 2.5 times lower than that of the short first neighbor bond, but similar to the force constants of the second neighbor bonds. These results are compared to those of first and higher neighbor bonds in metallic Cu, Ge with a classical covalent bonding and GeTe, thus contributing to the understanding of bonding in Sb as an elemental electron rich system.

DS 15.2 Thu 10:45 A 060

Atomic-scale characterization of Cu-Te phases prepared using focused ion beam and thermal heating — •Nils Braun[1], Vladimir Roddatis[2], Sonja Cremer[1], Hagen Bryja[1], Lennart Voss[3], Lorenz Kienle[3], and Andriy Lotnyk[1] — [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

Cu-Te phases are interesting for thermoelectric applications. However, their crystal structure is still under debate. In this work, we prepared different nanoscale Cu-Te phases from the Cu - Sb_2Te_3 system using FIB and thermal treatment. Epitaxial or polycrystalline Sb_2Te_3 thin films are grown on p-type Si (111) and SiO_2 coated wafers, respectively, by pulsed laser deposition. A standard cross-section FIB preparation method is employed and the lamellae are investigated using advanced TEM methods and XRD.

The formation of van der Waals bonded Cu-Te phases consisting of bi- and tri-layers of Te is observed in epitaxial and polycrystalline samples. The lattice parameters and position of Cu and Te atoms in the resulting phases are determined from atomic-resolution STEM and HREELS images. The crystal structure of the bilayered phase was identified as trigonal Cu_7Te_4 and orthorhombic/tetragonal Cu_3-xTe_2. Moreover, crystal defects such as dislocations were observed in the thin films.

We acknowledge P. Hertel and A. Mill for their support and financial support by the German Research Foundation (DFG 448667535).

DS 15.3 Thu 11:00 A 060

Switching of GeTe-Sb_2Te_3 multilayers by infrared femtosecond laser pulses — •Sonja Cremer[1], Martin Ehrhardt[1], Pierre Lorenz[1], and Andriy Lotnyk[1,2] — [1]Leibniz Institute of Surface Engineering, Leipzig, Germany — [2]Laboratory of Infrared Materials and Devices, Ningbo University, China

By phase change material multilayers (MLs) current drawbacks as resistance drift of Ge-Sb-Te thin films for neuromorphic computing may be tackled. This way MLs can help to unleash the full potential of the technologys advantageous characteristics like multilevel cell (MLC) operation. Switching is performed by electric or optical pulses, significantly changing the resistance and reflectivity of the thin film.

Here, we switched PLD grown 30 nm periodic GeTe-Sb_2Te_3-MLs using a 1030 nm laser with 260 fs pulse duration. The laser was part of an optical pump-probe setup to directly monitor reflectivity changes. Successful multiple switching was checked by light microscopy. Follow up SEM and TEM analysis were used to characterize the microstructure evolution. Switching between amorphous and fully crystalline state was found to go along with significant change in reflectivity (~20%). Besides, multilevel crystallization states with nonlinear reflectivity evolution were observed.

Thus, GeTe-Sb_2Te_3-MLs are a potential candidate for MLC operation with a fixed laser wavelength and pulse duration.

We acknowledge financial support by the DFG (No. 445693080) and thank Mrs. A. Mill for FIB preparation.

DS 15.4 Thu 11:15 A 060

An on-chip micro-thermoelectric temperature-controller — •Qun Jin, Kornelius Nielsch, and Heiko Reith — Institute for Metallic Materials, IFW Dresden, Dresden, Germany

To extend Moore's law in modern microelectronics, multidimensional nanoelectronic integration and multifunctional component assembly have been greatly explored in recent years. However, these approaches will inevitably make precise temperature control for temperature-sensitive electronic components a major challenge. Therefore, it is important to integrate thermoelectric (TE) films [1-2] into high-performance micro-on-chip temperature controllers.

Here, we report an approach to integrating our freestanding TE films into an on-chip micro-temperature controller for thermal energy management in power electronics [3]. It can achieve more energy-efficient temperature control than our previous TE coolers [4-5]. A cooling temperature exceeding 44.5 K can be achieved using only 445 μW, which is two orders of magnitude lower than that required in microheaters. In addition, our on-chip TE temperature controller shows an ultra-fast cooling rate exceeding 2,000 K/s and excellent reliability of up to 1 million cycles. Our micro temperature controller opens new avenues in developing modern electronics with numerous promising applications.

References: [1] Q. Jin, et al. Nature Materials, 18, 62-68 (2019). [2] Q. Jin, et al. Advanced Materials, 35, 2304751 (2023). [3] Q. Jin, et al. under revision in Nano-Micro Letters. [4] G. Li, et al. Nature Electronics. 1, 555-561 (2018). [5] Q. Zhang, et al. Nature Electronics. 5, 333-347 (2022).

DS 15.5 Thu 11:30 A 060

Field Effect Control of Thermoelectric Effect in Semiconductor Thin Films — •Sunao Shimizu[1], Kazumoto Miwa[2], Kazuyasu Tokiwa[3], and Shimpei Ono[1] — [1]Toyama Prefectural University, Toyama, Japan — [2]CRIEPI, Kanagawa, Japan — [3]Tokyo University of Science, Tokyo, Japan

Thermoelectric energy conversion has recently regained an increased interest as a promising technology for renewable energy systems. It is highly required to investigate diverse semiconductors for developing thermoelectric modules with higher energy conversion efficiency. In this presentation, we report the systematic characterization of thermoelectric properties in WO3. We fabricated WO3 thin films by RF sputtering and applied an ionic liquid gating technique to precisely control the carrier density. Due to the high gate capacitance at the electric double layer [1], which is formed at the interface of WO3 and the ionic liquid, high density charge carriers were accumulated on the semiconductor surface by just applying several volts of the gate voltage. The temperature dependence of the sheet resistance in WO3 initially showed insulating behavior and was modified to be metallic by the ionic liquid gating. We also discuss the systematic change of the thermoelectric effect, showing the optimization of the thermoelectric power factor with changing the carrier density [2].

[1] S. Bisri, S. Shimizu, M. Nakano, Y. Iwasa, Adv. Mater. 29, 1607054 (2017). [2] S. Shimizu et al., Sci. Rep. 12, 7292 (2022).

DS 15.6 Thu 11:45 A 060

Imaging the Ettingshausen effect and cryogenic thermoelectric cooling in a van der Waals semimetal — •Tobias Völkl[1], Amit Aharon-Steinberg[1], Tobias Holder[1,2], Edan Alpern[1], Nasrin Banu[1], Arnab Pariari[1], Yuri Myasoedov[1], Martin Huber[3], and Eli Zeldov[1] — [1]1Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel — [2]School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel — [3]Departments of Physics and Electrical Engineering, University of Colorado Denver, Denver, Colorado

Attaining viable thermoelectric cooling at cryogenic temperatures is of major fundamental and technological interest for novel electronics and quantum materials applications. Here we develop nanoscale cryogenic imaging of a magneto-thermoelectric effect and demonstrate absolute cooling and an ultrahigh Ettingshausen effect in exfoliated WTe_2 Weyl semimetal flakes at liquid He temperatures. Application of a current and perpendicular magnetic field gives rise to cooling via generation of electron-hole pairs on one side of the sample and heating by their recombination at the opposite side. In contrast to bulk materials, the cooling process is found to be nonmonotonic in magnetic field and in device size. The derived model of magneto-thermoelectricity in mesoscopic semimetal devices shows that the cooling efficiency and the induced temperature profiles are governed by the interplay between sample geometry, electron-hole recombination length, magnetic field, and flake and substrate heat conductivities.

DS 16: Focus Session: 2D Transition Metal Carbides, Nitrides and Carbonitrides III (joint session DS/MM/O)

Properties: Catalysis & electrochemistry; physical properties

Time: Thursday 15:00–17:30 Location: A 053

Invited Talk DS 16.1 Thu 15:00 A 053

Heterogeneous catalysis with MXenes: the role of the surface passivating groups and the structural defects — •Alexey Fedorov — Department of Mechanical and Process Engineering, ETH Zürich, CH-8092 Zürich, Switzerland

Mo2CTx, two-dimensional (2D) molybdenum carbide of the MXene family (Tx are passivating surface groups), contains only surface Mo sites and is therefore a convenient model catalyst for structure-activity studies. For instance, the catalytic activity of Mo2CTx in Fischer-Tropsch (FT) synthesis increases when a Tx coverage is minimized, the latter achieved via reductive defunctionalization of Tx groups under H2. However, high temperature H2 treatment of Mo2CTx removes also ca. one third of the carbidic lattice carbon, yielding a 2D-Mo2C1-x material that is an active methanation catalyst. The removal of Tx species is also possible in the FT conditions (i.e., in the presence of CO), and this gives 2D-Mo2C without detectable carbon vacancies and Tx groups. 2D-Mo2C material, in contrast to 2D-Mo2C1-x, converts CO to diesel range alkanes. Other examples considered include dry reforming of methane, (reverse) water gas shift as well as electrocatalytic reactions (HER, NO3RR) of Mo2CTx:M, i.e., a material with dopant sites (M = Co, Fe) replacing Mo sites in the lattice of Mo2CTx.

DS 16.2 Thu 15:30 A 053

Pt-doped Ti3C2Tx and Mo2Ti2C3Tx MXenes for catalytic hydrogenation — •Yilong Yan[1], Franck Morfin[1], Stéphane Célérier[2], and Laurent Piccolo[1] — [1]IRCELYON, CNRS & Université Lyon 1, 69626 Villeurbanne, France — [2]IC2MP, CNRS & Université de Poitiers, 86073 Poitiers, France

Transition metal carbides can act as efficient metal-like catalysts or catalyst supports, and MXenes offer renewed possibilities to anchor metal atoms and promote catalytic performances. Herein, we report on the elaboration of Pt/MXene single-atom catalysts and their performance in CO2 and alkadiene hydrogenation reactions.

Anchoring of single Pt atoms is favorable at the surface of Ti3C2Tx and Mo2Ti2C3Tx MXenes. According to in situ XAS and XPS, Pt cations partially reduce upon thermal treatment at 400 °C in H2 flow, while forming bonds with surface M atoms of the MXene. This includes the probable location of Pt atoms at M vacancies or Pt-M substitution, consistently with STEM. In addition, XAS, XRD and TPR reveal MXene restructuring together with desorption of chemical intercalants and terminal groups.

While Ti3C2Tx is inactive, Mo2Ti2C3TX exhibits significant catalytic activity for both reactions. The addition of single Pt atoms on Ti3C2Tx leads to unusually high selectivity to 2-butene from butadiene hydrogenation [Mater. Today Catal. 2023, 2, 100010]. For CO2 hydrogenation, Pt/Ti3C2Tx shows a high Pt-molar activity and almost 100% selectivity to CO; Pt/Mo2Ti2C3TX is even more active, while methane and methanol are formed as minority products.

DS 16.3 Thu 15:45 A 053

Cobalt based MXene composites for the Oxygen Evolution Reaction — •Michelle Browne — Young Investigator Group Electrocatalysis: Synthesis to Devices, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, Berlin 14109, Germany

In the Electrocatalysis: Synthesis to Devices Group at HZB, our research is focused on combining MXenes and metal oxides to create the next generation Oxygen Evolution Reaction (OER) catalysts. Metal oxides are known to be active for the OER but lack high conductivity. On the other hand, MXenes are highly conductive but oxidise readily under several conditions due to its termination sites and don't contain OER active sites. To overcome these issues, we employ several strategies in our group to combine these two materials to make one material which is OER active and high conductive. Furthermore, by blocking the MXene termination sites with a metal oxide, this may lead to less oxidation of the MXenes structure. This presentation will focus on the development of Co-based MXene materials for the OER through various fabrication methods and combining Co with other metal oxide materials (e.g. CoCu and CoRu). The OER performance of the MXene/metal oxides composites compared to their parent materials will be discussed. We will also evaluate the various strategies to one another and how the initial activity and stability of the composite materials are affected.

15 min. break

Invited Talk DS 16.4 Thu 16:15 A 053

Ultrafast Photoexcitations in 2D MXenes — •Lyubov Titova — Worcester Polytechnic Institute, Worcester, MA, USA

MXenes are 2D transition metal carbides and nitrides with electronic properties that can be tuned by their chemistry and structure. Metallic-like conductivity, flexibility, high optical damage threshold and ease of processing owing to their hydrophilicity, make MXenes candidates for a host of electronic and optical applications. We use ultrafast optical and THz spectroscopic techniques to investigate the nature and behavior of photoexcitations in MXenes of different chemistries. We show that electronic and optical properties of MXenes can be engineered by choices of the transition metals and their order as well as by controlling the intercalants in the interlayer gaps. Furthermore, we demonstrate that MXenes with high free carrier density show promise as polarizers and tunable electromagnetic interference shields in the THz range.

DS 16.5 Thu 16:45 A 053

UV-to-IR Broadband Ellipsometry Characterization of Spray-Coated MXenes — •Andreas Furchner[1], Tetiana Hryhorchuk[2], Yury Gogotsi[2], and Tristan Petit[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Drexel University (Nanomaterials Institute), Philadelphia, USA

The chemical composition of MXenes determines whether they exhibit metal-, semi-metal- or semiconductor-like properties, which is important knowledge regarding optoelectronic applications. We employ broadband ellipsometry to characterize the optical and structural properties of spray-coated MXene layers of different chemical composition on silicon and glass substrates. Measuring from the deep-UV (200 nm) to the mid-infrared (25 μm) provides simultaneous access to the electronic and free-charge-carrier properties of the MXenes, as well as to their vibrational fingerprints. Furthermore, ellipsometry enables the quantification of layer thicknesses, roughnesses and film inhomogeneities. The results are corroborated by Vis microscopy and atomic-force-microscopy (AFM) measurements. The authors acknowledge support from the Federal Ministry of Education and Research in the framework of the project Catlab (03EW0015A/B) and funding from the U.S. National Science Foundation (Grant Number CHE-2318105, M-STAR CCI).

DS 16.6 Thu 17:00 A 053

2D to 3D weak localization dimensional crossover in $Ti_3C_2T_x$ MXene induced by thickness and defect engineering — •Sophia Tangui[1], Simon Hurand[1], Lola Loupias[2], Stéphane Célérier[2], Ayoub Benmoumen[1,3], Philippe Moreau[3], Marie-Laure David[1], and Vincent Mauchamp[1] — [1]Université de Poitiers, ISAE-ENSMA, CNRS, PPRIME, Poitiers France — [2]Université de Poitiers, CNRS, IC2MP, Poitiers, France — [3]Nantes Université, CNRS, IMN, Nantes, France

Due to their hydrophilic properties and very good metallic electrical behavior, MXenes are promising materials for numerous applications, including transparent conductive thin films. Therefore, there is a need to unravel the transport mechanism involved in MXene multilayers. Although weak localization (WL) has been proposed as the dominating low-temperature transport mechanism in thin films, there have been however few attempts to model quantitatively temperature and magnetic field dependent resistivity measurements.

In this talk, we will focus on the dimensionality of the low-temperature transport mechanisms in spin coated thin films elaborated with the most-studied and metallic $Ti_3C_2T_x$ MXene. The influence of the thin film thickness on one hand and of defects introduced by ion

irradiation at different fluences on the other hand is studied by low temperature and magnetic field dependant resistivity measurements. The data are analyzed in the framework of both 2D and 3D models : we will demonstrate a non-trivial evolution between the two behaviors and discuss the validity of both models.

DS 16.7 Thu 17:15 A 053

Non-Covalent Functionalized Schottky Interface at Ti3C2Tx/c-Si Van der Waals Heterojunction — •Eloi Ros Costals, Sergio Giraldo, Marcel Placidi, Cristobal Voz, Joaquim Puigdollers, Edgardo Saucedo, Zacharie Jehl Li Kao, and Kunal Tiwari — Electronics Engineering Department, Polytechnic University of Catalunya (UPC), Barcelona Spain

Synergistic interaction between 2D materials and organic molecules presents an additional dimension for tuning their intrinsic properties. Herein, we aim to finely tune the work function of 2D Ti3C2Tx MXene by introducing ultrathin interlayers of organic dipoles (O.D.) with a defined dipole moment value. Interface engineering is achieved through the inclusion of poly(ethylene)amine (PEI 0.1%) and third generation poly(amido-)amine (PAMAM G3), between the Ti3C2TX and c-Si. Charge transport properties of the fabricated Schottky diodes with a structure of c-Si/O.D./Ti3C2TX were evaluated through systematic analysis of the I-V and C-V characteristics. Our investigations reveal that diodes featuring O.D. as interlayers exhibit substantially reduced reverse saturation current density (J0) and enhanced built-in potential (Vbi). We also report a significant reduction in the work function value of Ti3C2Tx from 5.8 eV to 4.2 eV for Ti3C2Tx/PEI 0.1% and 3.3 eV for Ti3C2Tx/PAMAM-G3 heterostructures. On the basis of inferences drawn from photoemission spectroscopy we ascribe this to formation of oriented interfacial dipoles at the Ti3C2Tx/O.D. interface. Our study introduces an innovative approach for precisely controlling the work function of Ti3C2Tx through the incorporation of O.D.

DS 17: Organic Thin Films, Organic-Inorganic Interfaces

Time: Thursday 15:00–16:30 Location: A 060

DS 17.1 Thu 15:00 A 060

Thin Film Growth Simulation Study of Diindenoperylene on $aSiO_2$ — •Philipp Elsässer and Tanja Schilling — Institute of Physics, University of Freiburg, Germany

The understanding of film growth mechanisms is of high technological importance for growing single crystals, coating surfaces, and film production. By now there is a good understanding of the processes involved in the growth of films consisting of spherical objects, like atoms. In contrast, films of elongated molecules behave with respect to some of their properties in different ways due to their additional rotational degrees of freedom.

The organic semiconductor Diindenoperylene (DIP) is a candidate for organic solar cells or OLEDs. We have investigated an amorphous SiO_2 ($aSiO_2$) substrate with DIP molecules deposited on the surface. For this, we have performed MD simulations to study the clustering of few DIP molecules on $aSiO_2$, as well as the molecular orientation in larger groups of DIP molecules.

DS 17.2 Thu 15:15 A 060

Towards measuring charge transfer in hybrid structures of sub-monolayer dye films on 2D materials — •Tim Völzer[1,2], Erik von der Oelsnitz[1,2], Julian Schröer[1], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institute of Physics, University of Rostock, Germany — [2]Department "Life, Light & Matter", University of Rostock, Germany

Coating transition metal dichalcogenides (TMDCs) with dye molecules creates hybrid structures offering a playground for ultrafast charge (or energy) transfer exploitable for optoelectronics. Typically, nanometer molecular films are applied to roughly match the crystal density of states. In this case, however, interfacial transfer processes compete with intermolecular interactions and the dynamics may be limited by diffusion towards the interface. Thus, we apply monomeric dye coatings, where the molecules lie far from and do not interact with each other. We perform transient absorption spectroscopy aiming for the ultrafast hole transfer from the dye Perylene Orange (PO) towards monolayer tungsten diselenide and the electron transfer in the reverse direction. As a reference sample, we use PO on hexagonal boron nitride, where no charge or energy transfer can occur and the slow dynamics of the isolated molecules is represented.

DS 17.3 Thu 15:30 A 060

Ab-initio study on mixed donor-acceptor adlayers: Structure, stoichiometry and electrostatic potential of F4TCNQ and 1H,1 H-[4,4]bipyridinylidene on Cu (111) — •Richard Berger and Oliver Hofmann — Petersgasse 16, 8010 Graz, TU Graz: Institut für Festkörperphysik

Adlayer patterns formed from heterogenous molecular species on a substrate surface are of great interest, especially in the case of 2-dimensional donor-acceptor patterns adsorbed on metal surfaces. Such adsorbed donor-acceptor patterns exhibit various remarkable characteristics, such as their ability to form two-dimensional charge density waves or the possibility of tuning the electron injection barrier at the interface via the stoichiometry of the mixed adlayer. Here, we computationally investigated the exemplary donor-acceptor system of F4TCNQ and 1H,1 H-[4,4]bipyridinylidene on the Cu (111) surface. We predict the thermodynamically stable adlayer structure for different mixing stoichiometries. This allows us to forecast the tunability of the on-surface stoichiometry and structure via the gas phase concentration ratio during the deposition process. Using these predictions, we explore how the complex electrostatic potential of the donor/acceptor mixture affects the barriers for charge injection into subsequent layers.

DS 17.4 Thu 15:45 A 060

Influence of Electrostatic Forces: Molecular Packing in 2D and 3D Films — •Jan Vincent Schreiber, Maximilian Dreher, and Gregor Witte — Philipps-Universität Marburg, Molekulare Festkörperphysik, 35032 Marburg, Germany

While packing motifs and crystal structures of van der Waals-bound molecular solids are essentially determined by an interplay of London dispersion and electrostatic forces, the latter often receives only little attention. Using the model system 5,7,12,14-Pentacenetetrone as an example, we use STM measurements to demonstrate the formation of different packing motifs in monolayer and bilayer films on graphite, which can be well explained by optimized electrostatic interactions in two and three dimensions, respectively. This knowledge then enables optimization of growth and the production of highly ordered strain-free films through the application of specific temperature protocols upon growth that abolish the initially formed 2D seed layer structure and yield very smooth, crystalline films with the bulk structure while avoiding dewetting that often occurs at higher temperatures. This result highlights the importance of accurately understanding interfacial properties to obtain crystalline molecular functional films.

DS 17.5 Thu 16:00 A 060

Polarized Raman Imaging of *para*-Hexaphenylene Nanoaggregates — •Frank Balzer[1], Roland Resel[2], and Manuela Schiek[3] — [1]Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark — [2]Institute of Solid State Physics, Graz University of Technology, Graz, Austria — [3]Center for Surface- and Nanoanalytics (ZONA), Johannes Kepler University, Linz, Austria

Organic molecular beam deposition of *para*-hexaphenylene (p6P) onto poly-crystalline platinum results in the formation of unique nanoaggregates, predominantly as nanofibers and ribbons. Atomic force microscopy reveals intricate morphological differences. Grazing incidence X-ray diffraction validates multiple crystalline contact faces, with a preference for crystallographic contact planes where molecules are oriented parallel to the substrate surface. No evidence of in-plane templating effects is observed. Uniform and varying optical extinction angles in birefringent aggregates suggest a complex aggregation process. Raman microscopy indicates that the molecular orientation within the aggregates is generally perpendicular to the long aggregate axis, aligning with the aggregate orientation. This finding is significant for applications leveraging p6P's polarized emission properties, such as in photonic and optoelectronic devices.

DS 17.6 Thu 16:15 A 060

Formation of CoS_x in the tribological taper junction of

hip implants — •Adrian Wittrock[1], Christian Beckmann[1], Markus A. Wimmer[2], Alfons Fischer[2,3], Christian Liebscher[4], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund University — [2]Department of Orthopedic Surgery, Rush University Medical Center, Chicago, USA — [3]Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH — [4]Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH

Within an artificial hip joint gross slip fretting corrosion occurs, leading to the formation of inorganic-organic tribomaterial which contains compounds of the human body fluid and wear particles from the implant materials. However, little is known about tribo-chemical and -structural processes and the types of organometallic species formed within hip-implant taper junctions. Using confocal Raman microscopy, we show that the tribological fretting gives rise to a denaturation of the albumin, associated with a breaking of sulphur bonds, so that - in turn - sulphur ions are released and react with cobalt ions from the Co-alloy of the hip implant. A thin tribofilm of amorphous/nanocrystalline CoS_x is thus formed, covering approximately 12.2 % of the fretting track of the CoCr29Mo6C0.03 surface.

DS 18: Optical Analysis of Organic Thin Films

Time: Thursday 17:00–17:45 Location: A 060

DS 18.1 Thu 17:00 A 060

The Impact of solution processing on the optoelectronic properties of TADF emitters — •Anatolii Kuimov — University of Bayreuth, Bayreuth, Gemany

Thermally Activated Delayed Fluorescence (TADF) emitters are crucial for achieving 100% efficiency in OLEDs, utilizing reverse intersystem crossing (RISC) to convert non-emissive triplet states into highly emissive singlet states. Our study focuses on DMAC-TRZ, showcasing promising TADF properties in diverse configurations. We explored film processing's impact on photophysical parameters and RISC rates.

Post-processing, involving temperature and solution treatments, proved instrumental in fine-tuning the RISC rate and enhancing the film's ordering* one of the pivotal factors in the photophysics of TADF materials. Moreover, our experiments on DMAC-TRZ films revealed these processes' surprising capability to adjust both parameters significantly. Additionally, the investigation demonstrated that the glass transition temperature of the emitter is less significant compared to the material's melting point during temperature annealing.

In conclusion, film processing and post-processing methodologies effectively improved film ordering and precisely adjusted RISC rates. These adjustments are critical for optimizing OLED efficiency.

This work was funded by the European Union

DS 18.2 Thu 17:15 A 060

Characterisation of thin layers of Polydopamine used as functional coatings in X-Ray optics. — •Andreas Hertwig[1], Elena Ermilova[1], Vincenzo Cotroneo[2], Eugenio Gibertini[3], Eva Stanik[4], and Thorsten Döhring[4] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM) — [2]INAF - Osservatorio Astronomico di Brera — [3]Politecnico di Milano — [4]TH Aschaffenburg

Polydopamine (PDA) is a biological / biomimetic polymer which has spiked considerable interest in recent years. Its monomer is an important neurotransmitter and it is one of the strongest glues produced by biological organisms. Polydopamine is a candidate for several applications, mainly in the field of biology and medicine, but also - recently - for layer coatings with optical, electrical, and mechanical function.

In this work, we investigate PDA layers intended as reflectivity enhancers for mirror surfaces in X-ray astronomical observatories. It has previously been shown, that such X-ray telescopes can be improved by a coating of PDA in the thickness range of several nm. Accurate thickness determination is required to monitor and optimise the coating process. We use spectroscopic ellipsometry to determine first the dielectric function of the polydopamine layers using model coatings of sufficient thickness. This data is then used to accurately determine the layer thickness of much thinner PDA layers. This study resulted in data on the thickness and dielectric function of PDA layers that could lead to a better understanding of the correlation of layer thickness and layer properties depending on the process parameters.

DS 18.3 Thu 17:30 A 060

Correlating Optical Transitions and the Selective Enhancement of Vibrational Modes in the Different Crystalline Phases of Semiconducting Discrete Oligomers — •Alexander Ehm, Rukiya Matsidik, Lukas Hertling, Michael Sommer, and Dietrich R. T. Zahn — TU Chemnitz, Chemnitz D-09107, Germany

The ever-growing zoo of organic semiconductors has a great potential to provide material-efficient, low-cost, and highly versatile alternatives, or supplementation, for (opto-)electronic applications. Recently developed naphthalene diimide- (NDI) and bithiophene- (T2) based, discrete oligomers avoid the typical disadvantages of polymeric semiconductors, such as batch-to-batch variation and high dispersity, while exhibiting opto-electronic properties similar to their polymeric counterparts [1]. Excitation-dependent Raman spectroscopy of the well-studied polymer P(NDI2OD-T2) comprising the same molecular units as the discrete oligomers, indicated selective enhancement of certain Raman modes linked to polaron confinement [2].

In our studies, we investigate the selective enhancement of Raman modes using a multitude of excitations of the discrete NDI-T2-based oligomers in dependence on their annealing-induced crystallisation. The results are supported by density functional theory calculations and correlated with optical transitions as obtained from transmission spectroscopy and spectroscopic ellipsometry investigations.

[1] Matsidik et al. J. Am. Chem. Soc. 2023, 145, 8430
[2] Giussani et al. Macromolecules 2013, 46, 2658

DS 19: Members' Assembly

Time: Thursday 18:00–19:00 Location: A 053

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

DS 20: Poster II

Time: Thursday 18:00–20:30 Location: Poster D

DS 20.1 Thu 18:00 Poster D

MBE-Growth Optimization and Optical Switching of Sb_2Te_3/GST-124 Superlattices — •Lucas Bothe[1], Peter Kerres[1], Lukas Conrads[2], Thomas Taubner[2], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase change materials (PCMs) are promising candidates for future data storage and neuromorphic computing solutions. In these applications drastic property changes between the amorphous (covalent) and the crystalline (metavalent) phase are exploited to encode data. The practical disadvantage of PCMs is the high energy necessary to switch from the crystalline to the amorphous phase (RESET) due to the melt-quench step. Previous studies revealed that replacing a single-layer PCM, e.g. GST, by alternating layers of Sb_2Te_3/GST, called superlattices (SL), reduces the reset current by an order of magnitude.

Highly textured Sb_2Te_3/GST-124 superlattices were grown via Molecular Beam Epitaxy (MBE) and their structure was investigated with $\theta/2\theta$-scans. The structural investigation revealed that the grown superlattices coincidence with the targeted superlattice stoichiometry and periodicity indicating optimized MBE-growth. Furthermore, a laser switching set-up was used to locally switch the as-grown SLs to the amorphous phase. The laser switching results will be discussed regarding the energy efficiency of the superlattices in comparison with ordinary phase change materials.

DS 20.2 Thu 18:00 Poster D

Investigation of Ultrafast Carrier Dynamics in ScN Using Pump-Probe Time-Resolved Spectroscopic Ellipsometry — •Younes Slimi[1,3], Johannes Laurenz Wolf[1], Martin Zahradník[2], Shirly Espinoza[2], Mateusz Rebarz[2], Rebecca Petrich[1], Mohamed Bouafia[3], Jakob Andreasson[2], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany — [2]ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Za Radnici 835, 25241 Dolni Brezany, Czech Republic — [3]Applied Optics Laboratory, Institute of Optics and Precision Mechanics, University of Setif 1, 19000, Setif, Algeria

Scandium nitride (ScN) is a promising material for optoelectronic applications owing to its wide band gap, high melting point, and chemical stability. With a band gap exceeding 2 eV, ScN serves as a suitable semiconductor for optoelectronics. Further investigation is warranted to comprehensively characterize its dielectric function, which is crucial for device development. Spectroscopic ellipsometry (SE) and pump-probe time-resolved SE (tSE) are employed to unravel the dielectric properties of ScN thin films, encompassing optical absorption, refractive index, and dielectric constant. Our findings reveal transient features in the dielectric function, shedding light on ultrafast carrier dynamics and relaxation processes. This comprehensive analysis advances our understanding of the material's fundamental behavior.

DS 20.3 Thu 18:00 Poster D

Design of lithium niobate on silicon surface acoustic waveguide for hybrid integrated phononic circuits — •Matthias Volz, Emeline Denise Sophie Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

Surface acoustic waves (SAWs) have proven to be effective in the control and manipulation of elementary excitations in condensed matter [1, 2]. In particular, SAWs have been efficiently used to interact with spin waves in magnetic thin film, which shows great potential for the realization of novel microwave devices [3]. In this work, the design of a lithium niobate on silicon (LNoSi) phononic waveguide is presented. The localization of the SAW propagation inside a phononic waveguide will enhance the coupling to hybrid quantum mechanical systems, such as spin waves. Furthermore, the used LNoSi platform offers many other advantages such as high piezoelectric coupling, the capability of photonic waveguiding in addition to the phononic modes, as well as the possibility of non-linear optics. The fundamental phononic waveguide modes determined by the waveguide geometry will be simulated using finite element methods and the phononic dispersion will be studied by varying the waveguide width and height. [1] Delsing et al., J. Phys. D: Appl. Phys. 52(35):353001 (2019) [2] Bühler et al., Nat. Commun. 13:6998 (2022) [3] Küß et al., Phys. Rev. B 107:024424 (2023)

DS 20.4 Thu 18:00 Poster D

Proton exchange on thin-film lithium niobate — •Maranatha Andalis, Ioannis Caltzidis, Oscar Camacho Ibarra, Hermann Kahle, Tobias Henksmeier, and Klaus D. Jöns — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn

Lithium niobate-on-insulator (LNOI) is an ideal platform for integrated optics due to its strong electro-optical and acousto-optic properties, wide transparency window, and relatively high refractive index. However, the fabrication of low-loss LNOI waveguides, attributed to the redeposition of by-products, remains a challenge today. One way to overcome this challenge is to replace lithium ions with protons, which can reduce the redeposition during dry etching. Although proton exchange has been utilized previously for bulk lithium niobate, studies on its application in thin films are not fully clarified. In this study, an x-cut LNOI was used to investigate proton exchange. The results will provide an overview of the most recent discoveries.

DS 20.5 Thu 18:00 Poster D

Growth and Characterisation of V_2O_5 and VO_x Phase Mixtures for Memristive Device Applications. — •Aisling Hussey, Brian Walls, and Igor Shvets — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

Vanadium oxides exhibit a range of oxidation states, from +3 to +5. Many of these states have metal-insulator transitions, which makes them candidate materials for memristive devices and resistive random access memory. V_2O_5 is the highest oxidation state and is a semiconductor with no metal-insulator transition. It can be reduced to form regions of V_6O_{13} and VO_2. The formation of these phases in a reduced single crystal leads to a reduction in resistance, as a conductive path through these phases is formed. [1] This work aims to investigate whether conducting filaments of these phases will form in V_2O_5 and reduced mixed phase thin films. V_2O_5 and mixed phase VO_x films have been grown using magnetron sputtering. The films have been structurally characterised using XRD and x-ray reflectivity, and electrically characterised by resistance measurements. Electric field driven reduction and formation of conducting filaments will be investigated and characterised using electrical measurements. The films will be structurally characterised following filament formation, to identify phases present in the conducting filament.

[1] Walls, Brian, et al. "VO_x Phase Mixture of Reduced Single Crystalline V_2O_5: VO_2 Resistive Switching." Materials 15.21 (2022): 7652.

DS 20.6 Thu 18:00 Poster D

Watching hydrogen diffusion into Lutetium thin films with thin Pd cap layers — •Zahra Hojjati[1,2], Harald Giessen[1,2], and Philipp Flad[1] — [1]4th Physics Institute — [2]Stuttgart Research Center of Photonic Engineering

Hydrogenated Lutetium is one of the materials that might have a potential to be used as high-temperature superconductor under high pressure. Recently three have been reports that the system Lu-H-N undergoes a phase transition to blue when hydrogenated, and unconfirmed reports indicate superconductivity. We therefore investigate hydrogen-lutetium interactions and the dynamics of hydrogen diffusion within lutetium, which is influenced by the ambient temperature, the crystal structure and the hydrogen concentration. Hydrogen diffusion in metals involves interstitial diffusion through the lattice and surface absorption. We use samples that consists of a thin Lutetium film with a stripe of Palladium as a catalyst on top. They were placed in a gas cell with 10% H_2 in N_2. The sample was heated to 70-80 degrees Celsius in the presence of H_2. The Lutetium-Palladium surface is getting dark within minutes. The color in Lutetium close to the Pd changes to blue, and this hydrogenation front advances over hours and days. Eventually, the Lutetium-Pd surface is transformed from black to brown, exhibiting cracks. We analyze the progression of the blue hydrogenation front in Lutetium was measured, and our evaluation

indicates a drift rather than a diffusion process. We determine drift velocity and the detailed hydrogenation dynamics, which is important for advancements in energy storage technology.

DS 20.7 Thu 18:00 Poster D

Racetrack memory devices based on freestanding thin films — •Ke Gu, Binoy Krishna Hazra, Yicheng Guan, Peng Wang, Andrea Migliorini, Hakan Deniz, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

One of the most promising future memory devices is magnetic racetrack memory (RTM), in which data is encoded in magnetic nanoobjects, e.g. magnetic domain walls (DWs), which are moved along nanowires by current pulses. RTM is promising due to its high packing density, low energy consumption and high speed. However, so far it has only been explored in two dimensions. Here, we show that by using a water membrane based freestanding technique, freestanding racetracks formed from heavy metal/ferromagnetic (HM/FM) and synthetic antiferromagnetic (SAF) heterostructures can be fabricated even in a 3D form. The structures and magnetic properties of freestanding heterostructures are largely preserved throughout the entire process. We show that the current induced DW motion in 3D racetracks formed from HM/FM heterostructures can be modulated by the local geometry and an efficient CIDWM can be realized in 3D racetracks formed from SAF heterostructures. In addition, we fabricate freestanding HM/FM racetracks without any buffer layer. We show that they have almost identical performance to the devices formed from conventional HM/FM heterostructures. As we demonstrated here, freestanding magnetic heterostructures thin films may enable future DW logic and 3D spintronic devices with high data capacity.

DS 20.8 Thu 18:00 Poster D

Evaluation of thin Pd layers used in a sensor system for the continuous measurement of high hydrogen concentrations in a fuel cell — •Christopher Bickmann[1], Lucas Viriato[2], Peter Schwotzer-Uhlig[2], Christoph Meinecke[1,3], Danny Reuter[1,3], Thomas von Unwerth[2], and Harald Kuhn[1,3] — [1]Center for Microtechnologies, University of Technology Chemnitz, Chemnitz 09126, Germany — [2]Department of Advanced Powertrains, University of Technology Chemnitz, Chemnitz 09126, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz 09126, Germany

The focus of this study is to evaluate the potential use of thin palladium layers for integration within a sensor system designed for use in a hydrogen fuel cell and to enable continuous measurement of high hydrogen concentrations. The functional principle is based on an increase in electrical resistance caused by the diffusion of hydrogen atoms into the metal lattice of the palladium. The methodology used involves the production of these thin-film structures using lithographic processes, which include techniques such as lift-off processes and physical vapor deposition. The characterization of the electrical resistance as a function of hydrogen concentration, humidity and temperature is carried out in a specially designed test chamber. It can be shown that the structures enable a continuous and reproducible measurement of the hydrogen concentration, whereby the measuring range is dependent on the layer thickness. An outlook on a sensor prototype is given, which is to be tested under real conditions in the further course.

DS 20.9 Thu 18:00 Poster D

Floating-base OPBTs for non-volatile memories — •Amric Bonil and Hans Kleeman — TU Dresden, Germany

In an effort to follow the organic electronics trend with its advantages of flexibility, portability, low-power consumption and biocompatibility, new designs for an organic non-volatile memory are being investigated. These devices could make up a path toward in-memory computing applications based on organic transistors.

Organic Permeable Base Transistors (OPBTs) have already demonstrated their excellent performance regarding high current and speed, good On/Off ratios and gain [1]. Here we show that OPBTs with a supplementary floating base can be used as a medium-term memory device. The vertical device architecture with thin, naturally formed, passivated layers of aluminum oxide surrounding both bases allow for a very small program voltage (+3V) with a memory window of 0.7 V. A retention time of up to 10^5 s can be reached for a very simple fabrication process that could be further enhanced to allow for reversible behavior (erasing).

[1] E. Guo, F. Dollinger, B. Amaya, A. Fischer, H. Kleemann, *Adv. Optical. Mater.* 9, 2002058 (2021).

DS 20.10 Thu 18:00 Poster D

Electric-field induced SHG (EFISHG) in graphene? — •Jonas Woeste[1,5], Klaas-Jan Tielrooij[2,3], Sergey Kovalev[4], Nikola Stojanovic[5], and Michael Gensch[5,1] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany. — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST and CSIC, Campus UAB, Bellaterra, Barcelona, Spain. — [3]Department of Applied Physics, TU Eindhoven, Eindhoven, The Netherlands. — [4]Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [5]DLR - Institute of Optical Sensor Systems, Berlin, Germany.

High harmonics generation (HHG) allows to study the nonlinear THz properties of e.g. single layer graphene by means of THz emission spectroscopy which can be explained by a simple thermodynamic model. Recently our collaboration successfully showed that (i) the nonlinearity of graphene can be controlled over two orders of magnitude by applying moderate gate voltages in the sub-Volt regime and (ii) that a specifically designed grating-graphene meta-material enables further increase in the THz nonlinearity via plasmonic field enhancement. Therein we have focused on odd-order nonlinearities, since monolayer graphene is a centrosymmetric material, where even-order susceptibilities cancel out. As a next step we plan to investigate if an effective 2nd order nonlinearity can be efficiently generated by applying appropriate in-plane DC electric fields, thus breaking the inversion symmetry, such as what has recently been demonstrated and observed in GaAs. Preparations for this experiment and its feasibility are discussed.

DS 20.11 Thu 18:00 Poster D

2D Layer MOCVD Growth of GaS on Sapphire: Insights on the Mechanism using TPD, AES and XPS — •Stefan Renato Kachel[1,2], Robin Günkel[2], Leonard Neuhaus[1], Johannes Glowatzki[2], Lukas Erlemeier[1], Kassandra Zoltner[1], Florian Münster[1], Carsten von Hänisch[1], Kerstin Volz[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Germany — [2]Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Germany

The utilization of 2D layers of GaS with its ultraviolet bandgap holds promise for applications in solar-blind photodiodes and LEDs. However, the growth of these 2D layers poses a significant challenge, resulting in the formation of 3D Ga droplets covered by GaS instead of the desired single layers. There is a keen interest in understanding the growth mechanism of the metal-organic chemical vapor deposition (MOCVD) process to achieve a high yield of 2D layers. This study focuses on investigating the growth of the precursors di-tert-butylsulfide (DTBS), tri-tert-butylgallium (TTBGa), and the single-source precursor diethylgallium-2-(ethylthio)ethane-1-thiolate (DEGEET) on sapphire. In the absence of Ga atoms on the sapphire surface, DTBS desorbs intact without forming S layers or replacing substrate oxygen. Conversely, TTBGa allows the deposition of Ga atoms, even at significantly lower temperatures than those commonly used in MOCVD processes. DEGEET enables the deposition of thin layers of Ga and S on the sapphire surface at low temperatures. Refining such single-source precursors could pave the way to growing 2D GaS.

DS 20.12 Thu 18:00 Poster D

Growth, Structural and Mangetic Properties of High Entropy Perovskite ($La_{0.2}Nd_{0.2}Gd_{0.2}Sm_{0.2}Y_{0.2}$)$MnO_3$ Thin Films — •Maximilian Mihm, Aladin Ullrich, David Stein, Christian Holzmann, Helmut Karl, and Manfred Albrecht — Institute of Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

High entropy manganite-perovskites such as ($La_{0.2}Nd_{0.2}Gd_{0.2}Sm_{0.2}Y_{0.2}$)$MnO_3$ (LNGSYMO) are typically produced as a powder and can exhibit interesting magnetic properties. We have grown thin films of LNGSYMO via pulsed laser deposition on $SrTiO_3$ (001) (STO) at 700°C. X-ray diffraction data confirmed epitaxial growth of LNGSYMO. Wide-range reciprocal space mapping and electron backscattered diffraction revealed, that LNGSYMO has three different crystal orientations. LNGSYMO grows in two different out-of-plane directions (001) and (110). The (001) orientated crystals are rotated by 45° with respect to the substrate, while the (110) crystals are aligned either to the substrate lattice or are also rotated by 45°. Zero-field cooled and field cooled (FC) measurements revealed a magnetic transition temperature at around 38 K for LNGSYMO grown on STO. This is in good agreement with the magnetic measurements on corresponding powder samples. Below 25 K the rare earth elements couple antiferromagnetic

to the Mn, which is indicated by a decrease of the magnetization in the FC curve.

DS 20.13 Thu 18:00 Poster D

Microphase Separation in Thin Films of a Sphere Forming PS-*b*-PDMS Block-Copolymer — •Janna X. Friebel, Alexander Stratmann, Harikrishnan Venugopal, and Jörg K. N. Lindner — Nanopatterning - Nanoanalysis - Photonic Materials, Department of Physics, Paderborn University, Germany

According to the bulk phase diagram by Bates et al. [1], block-copolymers (BCP) with a combined Flory-Huggins-parameter $\chi N > 10$ can form ordered nanostructures even with small degrees of polymerization (N), enabling sub-10nm nanostructures suitable for applications like nanomasks in microelectronics [2]. However, the bulk phase diagram is not applicable to thin films because of interfacial energy effects.

This investigation focuses on BCP thin films of PS-*b*-PDMS with a high χ and NB/NA ≈ 0.25, expected to form a bulk-state bcc arrangement of PDMS spheres in a PS matrix. Spin-coated onto Si substrates with native oxide films, the films undergo microphase separation in a solvent vapor atmosphere. After etching of the PS phase, AFM and SEM investigations reveal lamellar structures or cylinders oriented parallel to the surface. The morphology of these features and their arrangements are observed to be highly sensitive to slight changes in layer thicknesses and annealing conditions.

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

[2] Y. Chen, S. Xiong, Int. J. Extrem. Manuf. 2 (2020) 032006.

DS 20.14 Thu 18:00 Poster D

Investigation of the atomic arrangement of ultra thin MVB films using LEED-IV — •Maximilan Buchta[1], Peter Kerres[1], Christoph Ringkamp[1], and Matthias Wuttig[2] — [1]Forschungszentrum Jülich — [2]RWTH Aachen

The metavalent bond (MVB) is a newly proposed type of bond, that is fundamentally different from the ionic, metallic or covalent bonds. For many materials that possess MVB, like sesquichalcogenides, monochalcogenides or pnictogens (e.g., Sb2Te3, GeTe or Bi) the atomic arrangement within the unit cell significantly changes with increasing film thickness. Ex-situ techniques like X-ray diffraction (XRD) can easily determine the atomic arrangement for films above 3 nm. Yet, alternatives are needed for thinner films. Emerging from the need to measure the effects in ultra-thin films, Low Energy Electron Diffraction Intensity vs Electron Energy (LEED-IV) curves of MBE grown films have been obtained. Using dynamical LEED theory, the atomic arrangement of thin films of metavalent solids has been determined for different film thicknesses. This analysis reveals significant changes of the atomic arrangement as compared to bulk samples.

DS 20.15 Thu 18:00 Poster D

Tuning the magnetic properties of Fe_3O_4 thin films driven by electric field — •Yifan Xu[1,2], Patrick Schoeffmann[3], Connie Bednarski-Meinke[2], Chenyang Yin[1,2], Steffen Tober[2], Asmaa Qdemat[2], Oleg Petracic[2,1], and Mai Hussein Hamed[2,4] — [1]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf, Germany — [2]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Faculty of Science, Helwan University, Cairo, Egypt

Tuning magnetic oxide phases at heterointerfaces is a compelling strategy for advancing spintronic and memristive device applications. Specifically for iron oxides, we have shown that we can tune the magnetic and electrical properties of thin films upon initiating a phase transition between magnetite, maghemite and wüstite. Here we show the preparation and characterization of epitaxial Fe_3O_4 thin films grown on TiO_2 - terminated Nb:$SrTiO_3$ substrates via pulsed laser deposition (PLD). We observe a change in the Verwey transition - a critical indicator of the oxygen content in the Fe_3O_4 films and in particular, the disappearance of the Verwey transition when positive electric field is applied. In addition, using X-ray Magnetic Circular Dichroism (XMCD), we observed a shift in the Fe Edge. This could be explained by oxygen diffusion through the interface leading to a reversible phase transition from Fe_3O_4(magnetite) to γ-Fe_2O_3(maghemite).

DS 20.16 Thu 18:00 Poster D

Analysis of 3D check board pattern formation in NiCoMnAl shape memory alloys with alternating austenitic and martensitic layers — •Dario Stierl, Andreas Becker, Laila Bondzio, Inga Ennen, and Andreas Hütten — Universität Bielefeld

NiMnX (X=Al,Ga,Sn,In) magnetic shape memory Heusler alloys are considered as promising materials for magnetocaloric cooling applications due to their magnetoelastic coupling near room temperature. The thermal hysteresis could be reduced in NiCoMnAl thin films with alternating active transforming austenitic layers and martensitic intercalations. The stoichiometry of these two layers is chosen in such a way that their thermal hysteresis does not overlap. In addition, a 3D check board pattern becomes visible in HRTEM cross section images if the austenite active layers and martensite intercalations possess similar thicknesses.

In this contribution we aim for an improved understanding of the 3D check board pattern formation. Therefore, we varied the number of the alternating layers in one series and changed the ratio between the thicknesses of the two different layers in a different series. Furthermore, we analyzed the samples with temperature dependent XRD measurements. Additionally freestanding films were prepared and measured.

DS 20.17 Thu 18:00 Poster D

Biocompatible High-Entropy Alloys Thin Films with Antibacterial Properties — •Anna Benediktová, Lucie Nedvědová, and Ján Minár — New Technologies - Research Centre, University of West Bohemia, Plzeň, Czech Republic

High-entropy alloys (HEAs) represent an intensively studied group of metallic materials. Due to their unique properties and their potential to be very stable, wear-resistant, and hard, in addition to the possibility of tailoring some of their properties, HEAs have also become the subject of study as biomaterials. Commonly used metal biomaterials for implants still have many drawbacks such as low wear and corrosion resistance or lack of antibacterial properties, which can even result in the loss of the implant. In the case of porous polymer implants used in maxillofacial and plastic surgery, there is excellent ingrowth of soft tissues, but not osseointegration, which could be solved by applying a suitable implant coating. To improve the surface properties, novel HEAs thin films, with various amounts of silver to achieve antibacterial properties, have been prepared by magnetron sputtering, and their structure has been determined using scanning and transmission electron microscopy. Various substrates have been used such as cp-Ti or HDPE.

DS 20.18 Thu 18:00 Poster D

Epitaxial CVD growth of MoS2 on sapphire — •Blagovest Napoleonov[1], Dimitrina Petrova[1,2], Daniela Karashanova[1], Peter Rafailov[3], Vladimira Videva[1,4], Velichka Strijkova[1], Dimitre Dimitrov[1,3], and Vera Marinova[1] — [1]Institute of Optical Materials and Technologies-BAS Sofia, Bulgaria — [2]South-West University "Neofit Rilski", Blagoevgrad, Bulgaria — [3]Institute of Solid State Physics-BAS, Sofia, Bulgaria — [4]Sofia University, Sofia, Bulgaria

We present the epitaxial growth of MoS2 on sapphire substrate using low-pressure CVD method. The research focuses on optimizing the growth conditions to achieve reproducible results and explores the potential of conventional epitaxy for synthesizing crystalline nanoclusters/flakes of MoS2. By performing targeted substrates surface modification, we successfully achieve the desired epitaxial growth as confirmed by HRTEM. This research contributes to the development of scalable and high-quality Transition Metal Dichalcogenide (TMD) growth techniques, for practical applications.

Acknowledgements This work is supported by the Bulgarian National Science Fund under the grant number KP-06-COST/15; Research equipment of distributed research infrastructure INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science; the European Regional Development Fund within the Operational Programme "Science and Education for Smart Growth 2014-2020" under the Project CoE "National Centre of Mechatronics and Clean Technologies" BG05M2OP001-1.001-0008-C01.

DS 20.19 Thu 18:00 Poster D

Low energy ion-solid interactions: a quantitative experimental verification of binary collision approximation simulations — •Hans Hofsäss[1], Felix Junge[1], Patrick Kirscht[1], and Koen van Stiphout[2] — [1]II. Physikalisches Institut, Universität Göttingen, Germany — [2]Department of Physics, KU Leuven, Belgium

Ultra-low energy ion implantation has become an attractive method for doping of 2D materials. The dynamic binary collision approximation

Monte Carlo program IMINTDYN [1,2] allows a reliable prediction of low energy implantation profiles and target compositional changes, as well as efficient simulation of high energy light ion scattering. To demonstrate the quality of these simulations, we present implantation of W ions into tetrahedral amorphous carbon with low (10 keV) and ultra-low (20 eV) energies and high resolution Rutherford backscattering spectrometry (HR-RBS) to analyze the W implantation profiles with[1]. The experiment is compared with a complete simulation of all aspects of ion-solid-interactions of the experiment using the IMINTDYN. A unique novel simulation option is the inclusion of the vacancy as target species with dynamic vacancy generation and annihilation. We find excellent agreement between simulated and measured HR-RBS spectra if vacancy formation is included.

[1] H. Hofsäss, F. Junge, P. Kirscht and K. van Stiphout, Material Research Express (2023) DOI 10.1088/2053-1591/ace41c

[2] H. Hofsäss and A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49-62

DS 20.20 Thu 18:00 Poster D

Growth study of the altermagnet MnTe — •Marco Dittmar, Hannes Haberkamm, Philipp Kagerer, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Next to ferromagnetism and antiferromagnetism, a new type of magnetic order, called altermagnetism, has recently been predicted and has since attracted great attention. It is characterized by antiferromagnetic spin alignment combined with rotational lattice symmetry. Based on a profound symmetry analysis, various materials have been predicted to exhibit this type of magnetic order, one of which is MnTe in its hexagonal NiAs-type crystal structure [1].
Here, we present a growth study of MnTe on different substrates based on molecular beam epitaxy. Using X-ray diffraction, atomic force microscopy and photoemission spectroscopy, we will discuss e.g. the influence of the growth parameters on the observed films and the effect of substrate-induced lattice strain on the resulting crystal phase.
[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 031042 (2022)

DS 20.21 Thu 18:00 Poster D

Fast simulation of ion beam analysis spectra using binary collision approximation — •Hans Hofsäss, Felix Junge, and Patrick Kirscht — II. Physikalisches Institut, Universität Göttingen, Germany

The dynamic binary collision approximation program IMINTDYN [1,2] allows a reliable prediction of ion solid interaction. We have extended the IMINTDYN program to efficiently simulate high energy ion scattering as well as ion induced nuclear reaction spectra. This includes RBS, LEIS, ERDA, coincidence ERDA, ERCS, NRA and SIMS. The optimization includes (i) adjustable mean free path of high energetic ions (ii) enforced large angle scattering with scattering cross sections stored in weight factors, and (iii) enhanced data handling to identify coincident scattering events. The program runs on a AMD Ryzen Threadripper PRO 5965WX workstation. Typical simulations with millions of projectiles are finished within 2-20 minutes, faster than the duration of the experiment. The simulations provide details of the spectra, like single, dual and multiple scattering events, energy versus depth information, isotope information etc. We present selected examples for He ion RBS [1], Low energy He ion scattering (LEIS) as well as non-Rutherford backscattering of MeV H ions.

[1] H. Hofsäss, F. Junge, P. Kirscht and K. van Stiphout, Material Research Express (2023) DOI 10.1088/2053-1591/ace41c

[2] H. Hofsäss, A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49

DS 20.22 Thu 18:00 Poster D

Influence of post-growth temperature treatment on the surface structure of ion-beam sputtered vanadium oxide — •Yan Ravil Wollenweber-Bienerth, Antonia Krieger, Martin Becker, Sangam Chatterjee, and Peter J. Klar — Institute of Experimental Physics I , Heinrich-Buff-Ring 16, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany

Thermochromic (TC) smart windows are a type of fenestration whose transmittance switches as a function of the ambient temperature. Vanadium dioxide (VO_2) is by far the most studied TC material. Its insulator-to-metal transition is correlated with a crystalline phase transition accompanied by the change of transmittance/reflectance in the infrared region. To grow crystalline vanadium oxide thin films, usually high substrate temperatures are necessary. In an industrial process, however, post-growth annealing may be more desirable than in-situ heating during the deposition process. Furthermore, a post-growth temperature treatment may allow for a reduction of the growth temperature. Moreover, not only the material's phase is crucial, but also the evolution of the surface morphology of the functional layers.

Here, we employ ion-beam sputter deposition (IBSD) for the growth of VO_x and investigate different annealing routes for obtaining VO_2. We show that there is a temperature dependence of layer thickness and surface morphology of vanadium oxide as well as of its phase transition on annealing atmosphere, annealing pressure and annealing time. Thus, post-growth annealing enables further tuning the material's properties.

DS 20.23 Thu 18:00 Poster D

Plasma enhanced pulsed laser deposition of metal nitride and oxide thin films Dual radio frequency plasma enhanced pulsed laser deposition of metal nitride and oxide thin films — Heman Bhuyan[1], Rodrigo Villegas[1], Valentina Ureta[1], Miguel Escalona[1], Maria Jose Retamal[2], Maria Jose Inestroza[3], José Ignacio Fernández[1], Loïk Gence[1], •Ulrich G. Volkmann[1], and Yayoi Takamura[4] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Facultad de Ingenieria, Universidad Finis Terrae, Santiago, Chile — [3]Comisión Chilena de Energía Nuclear, Santiago, Chile — [4]Department of Materials Science and Engineering, University of California Davis, CA, USA

In this work, physics and application of a plasma enhanced pulsed laser deposition (PEPLD) system using dual radio frequency (RF) source will be presented. The dual radio frequency (RF) source has an additional benefit of controlling the ion energy and ion flux independently only by tuning the low frequency (LF) and high frequency (HF) components, respectively. Electrical and optical diagnostics, including time-resolved images, optical emission spectroscopy, and interferometry have been used to study the physics behind this PEPLD configuration. The results obtained from the deposition of titanium nitride and titanium dioxide thin films will be correlated with the interaction between the laser plum and the background RF plasma at different experimental conditions. The PEPLD system has successfully used to fabricate wrinkled titanium nitride nanocomposite for robust bendable electrodes. Acknowledgements: ANID FONDECYT 1220359.

DS 20.24 Thu 18:00 Poster D

Non-destructive analysis for ScAlN based MEMS — •Rebecca Petrich[1], Younes Slimi[1], Hauke Honig[2], Daniel Glöss[3], Stephan Barth[3], Hagen Bartzsch[3], Raphael Kuhnen[4], Dietmar Frühauf[4], Rüdiger Schmidt-Grund[1], Stefan Krischok[1], and Katja Tonisch[1] — [1]TU Ilmenau, FG Technische Physik I, IMN MacroNano, 98693 Ilmenau — [2]TU Ilmenau, FG Werkstoffe der Elektrotechnik, IMN MacroNano, 98693 Ilmenau — [3]Fraunhofer Institute for Organic Electronics, Electron Beam and Plasma Technology FEP, 01277 Dresden, Germany — [4]Endress+Hauser SE+Co. KG, TTD Technologieentwicklung, 79689 Maulburg

ScAlN is an attractive alternative to traditional quartz- or lead-based piezoelectric materials due to its high piezoelectric coefficients and technological compatibility with MEMS processes. Non-destructive analysis is ideal for future system integration, as process and quality control can be carried out directly during production. Optical and spectroscopic methods are generally used for this, but these require an established material model, which is not available for new material compositions such as ScAlN, especially as they have to be adapted to different stoichiometries. In this contribution, ScAlN thin films are characterized by non-destructive methods such as EDX, XRD, Spectroscopic Ellipsometry and verified by established methods such as SEM, AFM and GDOES. The dielectric properties are investigated by means of plate capacitor structures using Pt, TiN and Ni as contact materials.

DS 20.25 Thu 18:00 Poster D

Understanding the thickness-dependent dielectric permittivity of oxide thin films — •Alessio Zaccone — University of Milan, Department of Physics, 20133 Milan, Italy — Institute of Theoretical Physics, University of Göttingen, Germany

The dielectric properties of thin films are of paramount importance in a variety of technological applications, from thin film capacitors and field-effect transistors to 5G technologies, and of fundamental importance for solid state research. In spite of this, there is currently no theoretical understanding of the dependence of the dielectric permittivity on the thickness of thin films. We develop a confinement model within

the Lorentz-field framework for the microscopic Langevin-equation description of dielectric response in terms of the atomic-scale vibrational modes of the solid. Based on this, we derive analytical expressions for the dielectric permittivity as a function of thin film thickness, in excellent agreement with experimental data of Barium-Strontium-Titanate (BST) thin films of different stoichiometry. The theory shows that the decrease of dielectric permittivity with decreasing thickness is directly caused by the restriction in k-space of the available eigenmodes for field-induced alignment of ions and charged groups.

DS 20.26 Thu 18:00 Poster D

Characterization of electrical and structural properties of ultrathin substoichiometric NiO_x films — •Tobias Pollenske, Laurenz Hüffmeier, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin, substoichiometric NiO_x films offer promising applications in electronics and optoelectronics. The electronic structure of these films, whith transition from conductive (x=0) to insulating (x=1) state, enables targeted control of electrical conductivity and opens up potential for switching elements in electronics and transparent conductive layers in optoelectronics. In addition to transparency in the visible spectral range, the antiferromagnetic nature of nickel oxide (x=1) and ferromagnetism of Ni (x=0) makes these layers interesting for applications in spintronics. The holistic research of these material properties aims to develop a deep understanding and lay the foundation for innovative electronic devices, optoelectronic devices and high-performance sensors.

Hence, in this work, ultrathin NiO_x films with varying stoichiometries ($0 < x < 1$) were grown on insulating MgO(001) substrates using reactive molecular beam epitaxy (RMBE). The investigation focused on the temperature-dependent conductivity and charge carrier density of these films. Additionally, the structural characteristics of the films were determined through XRR and (HE)XRD. Complementary insights into the chemical composition of the films for both near surface and bulk, were obtained by Soft XPS and HAXPES measurements, respectively.

DS 20.27 Thu 18:00 Poster D

Freestanding (K,Na)NbO_3 thin films grown by metal-organic vapor phase epitaxy — •Jeremy Maltitz, Saud Bin Anooz, Jens Martin, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Pulsed Laser Deposition (PLD) is one of the most suitable deposition techniques used to deposit heterostructures with sacrificial layer to obtain freestanding oxide thin films. However, it suffers from the low oxygen partial pressure and high energetic particle bombardment during film growth, typically leading to oxide films with high structural and compositional defect density which results in inferior functional properties for the oxide film. In contrast, Metal-Organic Vapor Phase Epitaxy (MOVPE) provides films with significantly lower defects density due to growth conditions at higher oxygen partial pressures and nearby thermodynamic equilibrium. Thus, the combination of PLD and MOVPE is a promising approach to realize freestanding complex oxide membranes with high structural quality. Specifically, the ferroelectric material (K,Na)NbO3 is interesting since its properties are crucially determined by the application of strain. Traditionally this is achieved by heteroepitaxial growth of (K,Na)NbO3 thin films on lattice-mismatched substrates. More flexibility however, is given by detaching the (K,Na)NbO3 film from its growth substrate and transfer on a flexible support. However, the growth of (K,Na)NbO3 directly on the sacrificial layer is challenging due to the hygroscopic properties of the Sr3Al2O6 material system, which have to protected by introducing a thin buffer layer on the sacrificial layer.

DS 20.28 Thu 18:00 Poster D

A time-domain perspective on the structural and electronic response in epitaxial ferroelectric thin films — •Matthias Rössle[1], Christelle Kwamen[1], Wolfram Leitenberger[2], Pedro Rojo Romeo[3], Bertrand Vilquin[3], Catherine Dubourdieu[1,4], and Matias Bargheer[2,1] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]Ecole Centrale de Lyon, Ecully, France — [4]Freie Universität Berlin, Berlin, Germany

Using synchrotron-based time-resolved X-ray diffraction and simultaneously measured electrical data, we investigate the frequency-dependent operando response of epitaxially grown $Pb(Zr_{0.48}Ti_{0.52})_3$ capacitors epitaxially grown on Silicon substrates in the frequency range $2 < \nu \leq 200$ kHz. We find that the electrical and structural hysteresis loops deform at high frequencies above 40 kHz, leading to a lower saturation polarization at high frequencies. We explain these observations in a time-domain perspective: The polarization and the structural motion within the unit cell are coupled to the strain along the *c*-axis by the piezoelectric effect. The solution of this coupled oscillator system is derived experimentally from the simultaneously measured electronic and structural data.

DS 20.29 Thu 18:00 Poster D

time-resolved x-ray diffraction studies on ferroelectric thin film — •rekikua alemayehu[1], david pesquera[2], matthias rössle[3], and matias bargheer[1,3] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Catalonia, Spain — [3]Helmholtz Zentrum Berlin, BESSY II, Berlin, Germany

Polarization switching in ferroelectrics involves the motion of atoms in the crystal structure. Time-resolved x-ray diffraction is a powerful experimental technique to study the structural changes that occur during this process. Here, we show the simultaneous structural and electrical response of a barium titanate epitaxial thin film during and after the application of electric field pulses with amplitudes above and below the coercive field of the ferroelectric film. We will discuss how the transient strain encodes the influence of imprint phenomena on the switching dynamics.

DS 20.30 Thu 18:00 Poster D

Room temperature reversible colossal volto-magnetic effect in all-oxide metallic-magnet/topotactic-phase-transition material heterostructures — •Sourav Chowdhury[1,3], Supriyo Majumder[2,3], Rajan Mishra[3], Arup Mandal[4,3], Anita Bagri[3], Deodatta Phase[3], Moritz Hoesch[1], Ram Choudhary[3], Satish Yadav[3], and Suman Karmarkar[3] — [1]DESY, Hamburg, Germany — [2]Northwestern University, IIIinois, USA — [3]UGC-DAE CSR, Indore, India — [4]IISC, Bengaluru, India

Multiferroic materials have undergone extensive research in the past two decades to produce a sizable room-temperature magneto-electric effect [1]. Here, we developed an innovative way is to tune the functional properties based on the tremendous modulation of electronics and magnetization by the electric field of the topotactic phase transitions (TPT) in heterostructures composed of metallic-magnet/TPT-material. The application of a nominal potential difference of 2-3 Volts induces gigantic changes in magnetization by 100-250% leading to colossal Volto-magnetic effect, which would be tremendously beneficial for low-power consumption applications in spintronics [2,3]. Switching electronics and magnetism by inducing TPT through applying an electric field requires much less energy, making such TPT-based systems promising for energy-efficient memory and logic applications.

[1] G. Catalan et al. Adv. Mater. 2009, 21, 2463, [2] N. A. Spaldin et al. Nat. Mater. 2019, 18, 203, [3] A. Bagri et al. ACS Appl. Mater. Interfaces 2013, 15, 18391.

DS 20.31 Thu 18:00 Poster D

Preparation and electrochemical characterization of laminar GO/WS_2 membranes — •Ann-Sophie Meyer, Yossarian Liebsch, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Ion-selective membranes are needed for various technical applications such as electrodialysis, fuel cells, desalination and biomedical applications. Nowadays, polymer membranes are mainly used for these applications, but the special properties of 2D materials offer the possibility to produce more efficient membranes. In particular, graphene oxide (GO) membranes are attracting a lot of interest from the scientific community.

In this work, stable GO membranes and GO membranes with an additional amount of WS_2 were prepared by vacuum filtration and tested for their morphology as well as ionic conductivity. It was found that ionic conductivity can be improved by incorporating WS_2 in the GO membranes, however, neither the exact WS_2 content nor a uniform distribution in the resulting membrane could yet be obtained.

Thus, the question of how the introduction of WS_2 into GO membranes changes their electrochemical properties and, in particular, increases their conductivity, could only be partially answered within our study.

In order to ensure a homogeneous distribution of WS_2, possibilities for optimization of the fabrication method will be discussed. Future experiments can then determine the WS_2 content for optimal ionic conductivity.

DS 20.32 Thu 18:00 Poster D

Epitaxial stabilization of perovskite ATeO3 thin films — •Andreas Herklotz[1], Florina Stefania Rus[2], David P Cann[3], and Kathrin Dörr[1] — [1]Institute for Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany — [2]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania — [3]Oregon State University, Corvallis, OR

Tellurium oxides of the form ATeO3 typically do not crystallize in perovskite structures. Here, we show that perovskite-like ATeO3 (A = Ca, Sr, Ba) thin films can be grown on perovskite single-crystal substrates via epitaxial stabilization. The films are stable with high optical bandgaps, low dielectric losses and high electric breakdown strength. Hysteretic dielectric behavior in SrTeO3 and BaTeO3 strongly suggest the presence of antiferroelectricity and ferroelectricity, respectively. These properties make perovskite tellurium oxides a possibly appealing class as thin film coating or insulator material in advanced microelectronics. Tellurium oxides constitute a largely unexplored class of materials that might show new and interesting functionalities in epitaxial thin film form. Our work encourages new work within this field.

DS 20.33 Thu 18:00 Poster D

Mapping the lateral homogeneity of semiconducting monolayer 2D polar Ag using spectroscopic imaging ellipsometry — •Ulrich Limberg[1], Jakob Henz[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua Robinson[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Muenster, Germany — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

2D polar metals are a novel family of atomically thin plasmonic quantum materials, which are synthesized by confinement heteroepitaxial growth (CHet)[1]. Hereby, metal atoms such as silver or gallium are intercalated between bilayer graphene and a silicon carbide substrate. In the case of 2D polar silver, a stable monolayer structure forms which has been shown to be an indirect bandgap semiconductor[2]. However, Raman imaging seems to indicate the existence of a second, possibly metallic, phase[3].

We investigated 2D polar silver samples of varying growth conditions via spectroscopic imaging ellipsometry, in order to access lateral inhomogeneities by modifications in the dielectric functions sensitive to different phases.

1 N. Briggs, et al. Nature materials 19.6 (2020): 637-643.
2 W. Lee, et al., Nano letters, 22(19) (2022): 7841-7847.
3 M. Wetherington et al., 2D Materials, 8.4 (2021): 041003.

DS 20.34 Thu 18:00 Poster D

Dielectric function of Rubi in static and lasing operation — •Noah Stiem, Younes Slimi, Clara Köhler, Stefan Krischok, and Rüdiger Schmidt-Grund — TU Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau

In a future study of the transient dielectric function of the classic laser material ruby by time-resolved spectroscopic ellipsometry (TRSE) we plan to investigate the influence of stimulated emission on the TRSE results and their analysis. Here we lay the groundwork by determining the steady-state dielectric function tensor of ruby samples via Mueller-matrix ellipsometry in reflection and transmission configuration. The data presented is not only necessary for the analysis of subsequent time-dependent measurements, but already allows insight into the changes of the dielectric function due to pump excitation. When pumping with a blue laser, the static dielectric function shows a change in intensity of the chromium states responsible for lasing at 692.80 nm and 694.25 nm caused by laser action in the material.

DS 20.35 Thu 18:00 Poster D

Optical Analysis of Sputtered $(IST)_{1-x}(SnTe)_x$ Thin Films — •Thomas Schmidt[1], Christian Stenz[1], Michael Dappen[1], and Matthias Wuttig[1,2] — [1]1. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Institute Green IT (PGI-10), Forschungszentrum Jülich, 52428 Jülich, Germany

Phase-change materials (PCMs) are characterized by a strong contrast in optical properties between amorphous and crystalline phases. Unlike other PCMs, crystalline In_3SbTe_2 (IST) shows metallic behavior. Therefore, IST arouses interest in nanophotonic applications. However, the optical property contrast is mainly limited to the infrared spectrum. Alloying IST with other compounds is an attempt to expand the optical contrast to the visible spectrum. One of those alloy-candidates is SnTe, which is characterized by a negative real part of the dielectric function $\epsilon = \epsilon_1 + i \cdot \epsilon_2$, a high maximum value of ϵ_2 at around 2.2 eV and the same rocksalt-like structure in the crystalline phase as IST. Metavalently bonded (MVB) materials, like SnTe, are characterized by significantly different properties compared with compounds employing one of the fundamental well-established bonding mechanisms (e.g. ionic, metallic, covalent). In order to link optical properties with chemical bonding, spectroscopic ellipsometry and Fourier transform infrared spectroscopy (FTIR) was performed on sputtered thin films of approx. 75 nm thick $(IST)_{1-x}(SnTe)_x$. From this, the dielectric function of the amorphous and crystalline samples can be extracted. The changes in the dielectric function ϵ of the crystalline phase can be assigned to a transition of chemical bonding from metallic to MVB.

DS 20.36 Thu 18:00 Poster D

Quantum Corrections to the Transport Properties in Thin Films of $BaPbO_3$ — •Alexander Schmid, Robert Bartel, Patrick Seiler, Thilo Kopp, and German Hammerl — Chair of Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

The paper reports on the characterization of transport properties of epitaxial $BaPbO_3$ thin films grown on $SrTiO_3$ by pulsed laser deposition, taken at low temperatures and high magnetic fields.

The electric resistance in these films shows deviations from classical transport behavior at low temperature due to dimensional effects and pronounced spin-orbit coupling. Such corrections to the classical electric resistance can be understood in the framework of weak localization and electron-electron interaction [1]. Considering both of these impurity-driven quantum effects is essential to quantitatively understand the electric transport in $BaPbO_3$ thin films [2].

Here, we present recent results regarding the influence of a systematical change of the oxygen background pressure during growth of $BaPbO_3$ thin films by pulsed laser deposition on the quantum corrections to the electric resistance at low temperatures [3].

[1] P. Seiler, R. Bartel, T. Kopp, G. Hammerl, Phys. Rev. B 100, 165402 (2019). [2] R. Bartel, E. Lettl, P. Seiler, T. Kopp, G. Hammerl, physica stat. sol. (b) 259, 2100154, (2021). [3] A. Schmid, Master's Thesis, University of Augsburg (2023).

DS 21: Optical Analysis of Thin Films

Time: Friday 9:30–12:15 Location: A 053

Invited Talk DS 21.1 Fri 9:30 A 053

Spotlight on Crystalline Textured Anilino-Squaraine Thin Films featuring Multiple Davydov Splitting and Charge Transfer Excitons — •Manuela Schiek — JKU Linz, Austria

Quadrupolar anilino squaraine dyes exhibit distinct excitonic signatures in their visible absorption spectra due to strong intermolecular interactions. These excitons are a result of the spatial arrangement of the molecular backbones, which is steered by non-chromophoric terminal functionalization patterns. They can be of predominantly Frenkel-excitonic nature [1] or are hybridized with intermolecular charge transfer [2] and may feature an extraordinary strong excitonic circular dichroism [3]. Polarized spectro-microscopy and imaging ellipsometry are implemented to study the linear dichroism of crystalline domains, which is a direct probe for the excitonic transitions. Combined with structural analysis the orientation of molecules is traced and the excitonic bands are assigned by modelling. Especially imaging ellipsometry allows determination of the complete dielectric tensor [4], from which a multiple Davydov splitting including a dark state can be deduced for the case of an orthorhombic polymorph containing multiple non-equivalent molecules within the primitive unit cell.

[1] Balzer, Breuer, Witte, Schiek. Langmuir 38 (2022) 9266. [2] Balzer, Hestand, Zablocki, Schnakenburg, Lützen, Schiek. J. Phys. Chem. C 126 (2022) 13802. [3] Gavazzi, Schumacher, Grisanti, Anzola, Di Maiola, Zablocki, Lützen, Schiek, Painelli. J. Mater. Chem. C 11 (2023) 8307. [4] Funke, Duwe, Balzer, Thiesen, Hingerl, Schiek J. Phys. Chem. Lett. 12 (2021) 3053.

DS 21.2 Fri 10:00 A 053

Theory of X-ray excitation of two-dimensional materials — Dominik Christiansen[1], Ivan Maliyov[2], •Joris Sturm[1], Malte Selig[1], Marco Bernardi[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, CA 91125, USA

In this contribution, we present a combined theory of X-ray Bloch - and Maxwell's equations to describe X-ray absorption experiments like XANES and EXAFS. Particularly crucial in the calculation of EXAFS spectra is a detailed knwoledge about the electronic structure and the electron - X-ray interaction matrix elements. In contrast to prior work, where a semi-empirical tight-binding approach was employed [1], we have improved our methodology by including *ab initio* electronic structure calculations. As a proof of principle we calculated the absorption spectrum of graphene which recovers now spectral signals missing in the previous approach [1].

[1] Christiansen, Dominik, et al., Physical Review Research 5.2 (2023): 023002.

[2] Christiansen, Dominik, et al., "Joint ab initio and Maxwell-Bloch approaches for the description of X-ray excitations of two-dimensional materials" **(in preparation)**

DS 21.3 Fri 10:15 A 053

Probing ultrafast dynamics employing a laser-driven broadband soft X-ray reflectometer — •Jasmin Jarecki[1], Martin Hennecke[1], Lutz Ehrentraut[1], Matthias Schnürer[1], Stefan Eisebitt[1,2], and Daniel Schick[1] — [1]Max-Born-Institut für Nichtlineare Optik & Kurzzeitspektroskopie, Berlin, Germany — [2]Institut für Optik & Atomare Physik, TU Berlin, Germany

Soft X-ray reflectometry (XRR) combines elemental and chemical sensitivity when hitting core-to-valence resonances, few-nanometer spatial resolution due to short X-ray wavelengths, and femtosecond temporal resolution when employing ultrashort sources. This allows probing of ultrafast dynamics of buried layers and across interfaces of stratified nanostructures. Here, we present a laboratory-based setup for time-resolved XRR, employing broadband soft X-ray pulses with energies ranging from 200 to 600 eV and pulse durations of 26 fs provided by a high harmonics generation (HHG) source. In contrast to synchrotron radiation or FEL sources, the quasi-continuous spectrum of the HHG offers efficient probing of broad spectra, e.g. across L-edges of transition metals, and of a large volume in reciprocal space in only a single acquisition. We benchmark our setup by probing laser-induced structural dynamics of a Mo/Si superlattice (SL). In very good agreement with simulations, we observe a shift of the 1st SL Bragg peak in reciprocal space probed at photon energies around 500 eV. Our results are an important step towards accessing also ultrafast electronic and magnetic dynamics in similar scattering experiments at such high photon energies outside of large-scale facilities.

DS 21.4 Fri 10:30 A 053

Synthesis, structure, and optical properties of Multi-Au capped Si nanoislands as a novel saturable absorber with a high modulation depth — Ali Karatutlu[1], Umut Taylan[1,2], •Zehra Gizem Mutlay[1], and Bülend Ortaç[1] — [1]UNAM–Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, 06800-Turkey — [2]Empa, Swiss Federal Laboratories for Materials Science & Technology, Laboratory for Advanced Materials Processing, Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland

This study demonstrates the first-time synthesis of multi-Au capped nanoislands and its potential as a new non-linear hybrid material. The synthesis was conducted by a vapor-liquid-solid mechanism using a subsequent laser ablation and plasma-enhanced vapor deposition. The results are promising for the use of this material in non-linear optics as a saturable absorber and potential mode-locker due to a relatively high-modulation depth reaching around 15% measured using Ti-sapphire femtosecond (fs) laser light with a wavelength at 800 nm. The hybrid saturable absorber consisting of metallic and semiconductor structures was initially characterized using UV-Vis-NIR absorption and reflection spectroscopy, scanning electron microscopy, and transmission electron microscopy studies followed by a power-dependent transmission measurement of an fs light.

15 min. break

DS 21.5 Fri 11:00 A 053

Exploring the Tunability of Phonon Properties in Ultra-Thin Bismuth Films — •Felix Hoff[1], Timo Veslin[1], Abdur Rehman Jalil[2], Peter Kerres[2], Jonathan Frank[1], Thomas Schmidt[1], Yazhi Xu[3], Dasol Kim[1], Riccardo Mazzarello[3], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Germany — [3]Dipartimento di Fisica, Sapienza University of Rome, Italy

In recent years, ultra-thin bismuth films have gathered attention for applications in thermoelectrics, ferroelectrics, and recently for topological applications, too. Our study focuses on the systematic exploration of ultra-thin bismuth films, utilizing advanced characterization techniques to unveil the intriguing changes in phonon properties as the layer thickness is reduced. Raman spectroscopy and optical fs pump probe spectroscopy were employed to measure phonon frequencies and lifetimes, exposing a complex interplay of factors influencing the observed hardening and softening of phonon modes. Additional investigations employ XRD, revealing structural modifications and distortions. DFT calculations unravel the intricate relationship between structural changes, chemical bonding, and optical properties. We determine the layer-thickness-dependent dielectric function, which show remarkable confinement effects. Epitaxially grown samples, detailed in a prior publication, ensure reproducibility. Motivated by achieving high-quality thin films, our work contributes to understanding the underlying mechanisms governing phonon properties in ultra-thin bismuth.

DS 21.6 Fri 11:15 A 053

Surface-Sensitive and Bulk-Suppressed Raman Scattering by Transferable Nanoporous Plasmonic Membranes — •Pietro Marabotti[1], Roman M. Wyss[1], Günter Kewes[1], Martin Frimmer[2], Karl-Philipp Schlichting[2], Markus Parzefall[2], Eric Bonvin[2], Martin F. Sarott[2], Morgan Trassin[2], Lala Habibova[1], Giorgia Marcelli[1], Marcela Giraldo[2], Jan Vermant[2], Lukas Novotny[2], Mads C. Weber[3], and Sebastian Heeg[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]ETH Zürich, Switzerland — [3]Le Mans Université, France

The Raman response of surfaces or thin films is often too weak to be detected and obscured by dominant bulk signals. Here we overcome this limitation by placing a transferable porous Au membrane (PAuM) on top of the surface of interest. Slot-like nanopores in the membrane

act as plasmonic slot antennas and enhance the Raman response of the surface underneath. The PAuM also suppresses the penetration of the excitation laser into the bulk, efficiently blocking the bulk Raman signal. Using graphene as a model surface, we show that these two effects increase the surface-to-bulk Raman signal ratio by 3 orders of magnitude. We find that 90% of the Raman enhancement occurs within the top 2.5 nm of the material, demonstrating truly surface-sensitive Raman scattering. To validate our approach, we analyze the surface of a $LaNiO_3$ thin film, observing a Raman mode splitting from the surface-layer, which is evidence that the surface structure differs from bulk. This shows that PAuM give direct access to Raman signals of surfaces and their structural properties.

DS 21.7 Fri 11:30 A 053

Thermal conductivitiy of hard-metal thin films microscopically resolved by Brillouin scattering — •Nils Denkmann[1], Donita Delijaj[1], Lasse Leukefeld[1], Nelson Filipe Lopes Dias[2], Finn Ontrup[2], Wolfgang Tillmann[2], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund — [2]Institute of Materials Engineering, TU Dortmund

Common procedures to measure the thermal conductivity of thin films are, e.g., the differential scanning calorimetry or the transient thermoreflectance. These methods predominantly provide macroscopic values and are not applicable to samples with complex geometries. To determine the thermal conductivity with micrometer spatial resolution and independently of the sample geometry as well as to understand the nanoscopic mechanisms alternative methods are needed. Here, we show how acoustic surface waves inside hard-metal thin films (e.g., TiAlN) are examined directly using Brillouin laser-light scattering. This method allows us to determine the thermal conductivity as function of the waves' propagation direction and the shear/Young's modulus. Spatial scanning is moreover exploited to correlate our microscopic acquisition with complementary macroscopic data. The results will provide a thorough insight into the effects of thermo-mechanical properties of hard-metal thin films.

DS 21.8 Fri 11:45 A 053

Scanning Reflectance Anisotropy Microscopy: Strain Mapping of Metasurfaces and Beyond — •Fabian Haake, Joan Sendra, Henning Galinski, and Ralph Spolenak — ETH Zurich, Zurich, Switzerland

A common failure mode of flexible electronic devices is catastrophic failure or device degradation due to mechanical strain, making accurate strain control a critical aspect in their design and characterization. Here, we introduce scanning reflectance microscopy (SRAM) as a broadband multi-material platform for strain mapping on the microscale. This multi-material optical platform serves not only to access microscopic strain distributions but also shows high phase sensitivity.

This technique provides a practical approach to mechanical characterization, yielding valuable insights into the mechanical behavior of diverse materials, including metamaterials, amorphous and crystalline semiconductors, and metals. The microscope's capability to generate diffraction-limited strain and phase maps enables a thorough analysis of materials properties without causing damage.

The capabilities of the technique are discussed on specific examples, such as strained metals and semiconductors as well as metasurfaces. Special emphasis is laid on the chance to apply this technique for in-situ studies and post-mortem analysis of fractured materials.

[1] J. Sendra, F. Haake, M. Calvo, H. Galinski, and R. Spolenak, Multi-Material Strain Mapping with Scanning Reflectance Anisotropy Microscopy, Adv Funct Materials, p. 2302179, Jun. 2023, doi: 10.1002/adfm.202302179.

DS 21.9 Fri 12:00 A 053

Exploring the optical constants of ruthenium (Ru) through EUV metrology:a study on thin films — •Samira Naghdi and Victor Soltwisch — Abbestraße 2-12, 10587 Berlin, Germany

This study presents a comprehensive investigation into the optical constants of ruthenium (Ru), focusing on thin films with a thickness of 30 nm. Employing Extreme Ultraviolet (EUV) metrology, our study investigates the spectral response of Ru across a wavelength range of 10 to 20 nm. The experimental setup involved measurements at varying angles, ranging from 2 to 88 degrees, to provide a thorough understanding of the material's optical behavior. The utilization of EUV metrology in this research not only ensures precision in wavelength selection but also offers a unique insight into the optical properties of Ru within the EUV spectrum. The study aims to contribute valuable data to the broader understanding of Ru's behavior, particularly in thin film applications, with potential implications for advancements in nanotechnology, optoelectronics, and other fields where ruthenium plays a crucial role. The results of this study not only contribute to the fundamental understanding of ruthenium's optical properties but also open avenues for further exploration and application in cutting-edge technologies.