Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls H14 and H17; Poster P3)

Invited Talks

DS 2.1	Mon	9:30–10:00	H17	**GaN-based power converters enabling talktive power** — •Marco Liserre
DS 2.2	Mon	10:00–10:30	H17	**Energy-efficient power electronics based on Gallium Nitride** — •Oliver Ambacher
DS 2.4	Mon	10:45–11:15	H17	**Potential of Aluminum Nitride for Vertical Power Electronics** — •Andreas Waag, Klaas Strempel, Lukas Peters, Christoph Margenfeld, Samuel Faber, Friedhard Römer, Bernd Witzigmann
DS 6.1	Mon	15:00–15:30	H17	**Novel high power device structures: Enabling compact and integrated power ICs** — •Elison Matioli
DS 6.2	Mon	15:30–16:00	H17	**Ab-initio investigations of V-pits and nanopipes in GaN** — •Liverios Lymperakis, Su-Hyun Yoo, Jörg Neugebauer
DS 6.4	Mon	16:15–16:45	H17	**Lateral and Vertical β-Ga_2O_3 Power Transistors for High-Voltage Applications** — •Kornelius Tetzner, Michael Klupsch, Karina Ickert, Ralph-Stephan Unger, Zbigniew Galazka, Ta-Shun Chou, Saud Bin Anooz, Andreas Popp, Joachim Würfl, Oliver Hilt
DS 14.1	Wed	9:30–10:00	H17	**Facet dependence of reconstructions at quantum material interfaces** — •Eva Benckiser
DS 14.3	Wed	10:15–10:45	H17	**Designing novel electronic phases at oxide interfaces from first principles** — •Rossitza Pentcheva

Invited Talks of the joint Symposium Frontiers of Orbital Physics: Statics, Dynamics, and Transport of Orbital Angular Momentum (SYOP)

See SYOP for the full program of the symposium.

SYOP 1.1	Mon	9:30–10:00	H1	**Orbital degeneracy in transition metal compounds: Jahn-Teller effect, spin-orbit coupling and quantum effects** — •Daniel Khomskii
SYOP 1.2	Mon	10:00–10:30	H1	**Orbital magnetism out of equilibrium: driving orbital motion with fluctuations, fields and currents** — •Yuriy Mokrousov
SYOP 1.3	Mon	10:30–11:00	H1	**Orbitronics: new torques and magnetoresistance effects** — •Mathias Kläui
SYOP 1.4	Mon	11:15–11:45	H1	**Orbital and total angular momenta dichroism of the THz vortex beams at the antiferromagnetic resonances** — •Andrei Sirenko
SYOP 1.5	Mon	11:45–12:15	H1	**Observation of the orbital Hall effect in a light metal Ti** — •Gyung-Min Choi

Invited Talks of the joint Symposium SKM Dissertation Prize 2022 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:15–10:45	H2	**Charge localisation in halide perovskites from bulk to nano for efficient optoelectronic applications** — •Sascha Feldmann

SYSD 1.2	Mon	10:45–11:15	H2	**Nonequilibrium Transport and Dynamics in Conventional and Topological Superconducting Junctions** — •Raffael L. Klees
SYSD 1.3	Mon	11:15–11:45	H2	**Probing magnetostatic and magnetotransport properties of the antiferromagnetic iron oxide hematite** — •Andrew Ross
SYSD 1.4	Mon	11:45–12:15	H2	**Quantum dot optomechanics with surface acoustic waves** — •Matthias Weiss

Invited Talks of the joint Symposium From Physics and Big Data to the Design of Novel Materials (SYNM)

See SYNM for the full program of the symposium.

SYNM 1.1	Mon	15:00–15:30	H1	**How to tackle the "I" in FAIR?** — •Claudia Draxl
SYNM 1.2	Mon	15:30–16:00	H1	**Beyond the average error: machine learning for the discovery of novel materials** — •Mario Boley, Simon Teshuva, Felix Luong, Lucas Foppa, Matthias Scheffler
SYNM 1.3	Mon	16:00–16:30	H1	**The Phase Diagram of All Inorganic Materials** — •Chris Wolverton
SYNM 1.4	Mon	16:45–17:15	H1	**Automated data-driven upscaling of transport properties in materials** — •Danny Perez, Thomas Swinburne
SYNM 1.5	Mon	17:15–17:45	H1	**Data-driven understanding of concentrated electrolytes** — •Alpha Lee

Invited Talks of the joint Symposium United Kingdom as Guest of Honor (SYUK)

See SYUK for the full program of the symposium.

SYUK 1.1	Wed	9:30–10:00	H2	**Structure and Dynamics of Interfacial Water** — •Angelos Michaelides
SYUK 1.2	Wed	10:00–10:30	H2	**A molecular view of the water interface** — •Mischa Bonn
SYUK 1.3	Wed	10:30–11:00	H2	**Motile cilia waves: creating and responding to flow** — •Pietro Cicuta
SYUK 1.4	Wed	11:00–11:30	H2	**Cilia and flagella: Building blocks of life and a physicist's playground** — •Oliver Bäumchen
SYUK 1.5	Wed	11:45–12:15	H2	**Computational modelling of the physics of rare earth - transition metal permanent magnets from $SmCo_5$ to $Nd_2Fe_{14}B$** — •Julie Staunton
SYUK 2.1	Wed	15:00–15:30	H2	**Hysteresis Design of Magnetic Materials for Efficient Energy Conversion** — •Oliver Gutfleisch
SYUK 2.2	Wed	15:30–16:00	H2	**Non-equilibrium dynamics of many-body quantum systems versus quantum technologies** — •Irene D'Amico
SYUK 2.3	Wed	16:00–16:30	H2	**Quantum computing with trapped ions** — •Ferdinand Schmidt-Kaler
SYUK 2.4	Wed	16:45–17:15	H2	**Breaking the millikelvin barrier in cooling nanoelectronic devices** — •Richard Haley
SYUK 2.5	Wed	17:15–17:45	H2	**Superconducting Quantum Interference Devices for applications at mK temperatures** — •Sebastian Kempf

Invited Talks of the joint Symposium Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence Applied to Real Materials (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Thu	15:00–15:30	H1	**Machine-learning-driven advances in modelling inorganic materials** — •Volker L. Deringer
SYES 1.2	Thu	15:30–16:00	H1	**Machine-Learning Discovery of Descriptors for Square-Net Topological Semimetals** — •Eun-Ah Kim
SYES 1.3	Thu	16:00–16:30	H1	**Four Generations of Neural Network Potentials** — •Jörg Behler
SYES 1.4	Thu	16:30–17:00	H1	**Using machine learning to find density functionals** — •Kieron Burke
SYES 1.5	Thu	17:00–17:30	H1	**Coarse graining for classical and quantum systems** — •Cecilia Clementi

Invited Talks of the joint Symposium Complexity and Topology in Quantum Matter (SYQM)

See SYQM for the full program of the symposium.

SYQM 1.1	Fri	9:30–10:00	H1	**The role of crystalline symmetries in topological materials: the topological materials database** — •Maia Vergniory
SYQM 1.2	Fri	10:00–10:30	H1	**Microwave Bulk and Edge Transport in HgTe-Based 2D Topological Insulators** — •Erwann Bocquillon, Matthieu C. Dartiailh, Alexandre Gourmelon, Hiroshi Kamata, Kalle Bendias, Simon Hartinger, Jean-Marc Berroir, Gwendal Fève, Bernard Plaçais, Lukas Lunczer, Raimund Schlereth, Hartmut Buhmann, Laurens Molenkamp
SYQM 1.3	Fri	10:30–11:00	H1	**Spectral Sensitivity of Non-Hermitian Topological Systems** — •Jan Carl Budich
SYQM 1.4	Fri	11:15–11:45	H1	**Topological photonics and topological lasers with coupled vertical resonators** — •Sebastian Klembt
SYQM 1.5	Fri	11:45–12:15	H1	**Spectroscopic Studies of the Topological Magnon Band Structure in a Skyrmion Lattice** — •Markus Garst

Sessions

DS 1.1–1.5	Mon	9:30–10:45	H14	**Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 1**
DS 2.1–2.4	Mon	9:30–11:15	H17	**Focus Session: Innovative GaN-based High-power Devices: Growth, Characterization, Simulation, Application 1**
DS 3.1–3.10	Mon	9:30–12:45	H36	**2D Materials 1 (joint session HL/CPP/DS)**
DS 4.1–4.3	Mon	11:00–11:45	H14	**Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 2**
DS 5.1–5.6	Mon	11:30–13:00	H17	**Organic Thin Films, Organic-Inorganic Interfaces**
DS 6.1–6.4	Mon	15:00–16:45	H17	**Focus Session: Innovative GaN-based High-power Devices: Growth, Characterization, Simulation, Application 2**
DS 7.1–7.12	Mon	15:00–18:30	H36	**2D Materials 2 (joint session HL/CPP/DS)**
DS 8.1–8.2	Mon	17:15–17:45	H38	**2D Materials 3 (joint session CPP/DS)**
DS 9.1–9.6	Tue	9:30–11:00	H14	**Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 3**
DS 10.1–10.3	Tue	9:30–11:30	H17	**Gaede Prize Talks**
DS 11.1–11.8	Tue	9:30–12:45	H34	**Focus Session: Quantum Properties at Functional Oxide Interfaces 1 (joint session HL/DS)**
DS 12.1–12.8	Tue	9:30–12:00	H36	**2D Materials 4 (joint session HL/CPP/DS)**
DS 13.1–13.5	Wed	9:30–10:45	H14	**Thin Film Applications 2**
DS 14.1–14.4	Wed	9:30–11:00	H17	**Focus session: Quantum Properties at Functional Oxide Interfaces 2 (joint session DS/HL)**
DS 15.1–15.9	Wed	9:30–12:00	H36	**2D Materials 5 (joint session HL/CPP/DS)**
DS 16.1–16.4	Wed	11:00–12:00	H14	**Thin Film Applications 2**
DS 17.1–17.7	Wed	11:15–13:00	H17	**2D Materials 6 (joint session DS/CPP)**
DS 18.1–18.4	Wed	15:00–16:00	H14	**Thin Oxides and Oxide Layers 1**
DS 19.1–19.4	Wed	15:00–16:00	H17	**2D Materials 7 (joint session DS/CPP)**
DS 20.1–20.52	Wed	16:00–18:00	P3	**Poster**
DS 21.1–21.4	Thu	9:30–10:30	H14	**Layer Deposition (ALD, MBE, Sputtering, ...)**
DS 22.1–22.8	Thu	9:30–11:30	H17	**2D Materials 8 (joint session DS/CPP)**
DS 23.1–23.6	Thu	10:45–12:15	H14	**Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...)**
DS 24.1–24.4	Thu	11:15–12:15	H36	**2D Materials 9 (joint session HL/CPP/DS)**
DS 25.1–25.4	Thu	15:00–16:00	H14	**Transport Properties**
DS 26.1–26.4	Thu	16:15–17:15	H14	**Thin Oxides and Oxide Layers 2**
DS 27.1–27.9	Fri	9:30–12:00	H36	**2D Materials 10 (joint session HL/CPP/DS)**

DS 1: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 1

Time: Monday 9:30–10:45 Location: H14

DS 1.1 Mon 9:30 H14

Low-energy ion channeling in nanocubes — •Shiva Choupanian[1], Wolfhard Möller[2], Martin Seyring[1], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Helmholtz-Zentrum Dresden-Rossendorf

Focused ion beam (FIB) processing with low-energy ions has become a standard technique for the manipulation of nanostructures. Many underlying ion beam effects that deviate from conventional high-energy ion irradiation of bulk systems are considered today; however, ion channeling with its consequence of significant deeper penetration depth has been only theoretically investigated in this regime. We present here an experimental approach to determine the channeling of low-energy ions in crystalline nanoparticles by measuring the sputter yield derived from SEM images taken after irradiation under various incident ion angles. Channeling maps of 30 and 20 keV Ga+ ions in Ag nanocubes have been identified and fit well with the theory. Indeed, channeling has a significant impact on the transport of energetic ions in crystals due to the large critical angle at low ion energies, thus being relevant for any FIB-application. Consequently, the obtained sputter yield clearly differs from amorphous materials; therefore, it is recommended not to rely only on, e.g., ion distribution depths predicted by standard Monte-Carlo (MC) algorithms for amorphous materials.

DS 1.2 Mon 9:45 H14

Tuning the properties of thin films via disorder — •Alessandro Troglia[1], Jorik van de Groep[2], Anne de Visser[2], and Roland Bliem[1,2] — [1]Advanced Research Center for Nanolithography (ARCNL), Science Park 106, 1098 XG Amsterdam, The Netherlands (NL) — [2]Van der Waals-Zeeman Institute, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands (NL)

Structural disorder in thin films is often considered detrimental compared to the well-defined nature of epitaxial layers. However, some examples of amorphous thin films show superior properties such as better corrosion resistance, mechanical strength and catalytic performance. Here we investigate amorphous and crystalline CuZr thin films of identical composition. Grazing-incidence x-ray diffraction (GI-XRD) demonstrate that amorphous and crystalline CuZr thin films were achieved by varying the substrate temperature during deposition with pulsed laser deposition (PLD). The effect of disorder is clearly visible in the optical, transport and corrosion properties. The amorphous films are optically transparent in the visible, while polycrystalline films are dark and reflective. The temperature-dependent electronic transport changes its mode from a bad metal to a charge-hopping conductor with an increase in structural disorder. Moreover, we observe a higher oxidation resistance of amorphous CuZr thin films due to the absence of grain boundaries. These results pave the way to the synthesis of metallic thin films with superior and tunable properties via disorder for customizing materials properties to their technological applications.

DS 1.3 Mon 10:00 H14

Faster and lower dose X-ray reflectivity measurements enabled by physics-informed modelling and artificial intelligence co-refinement — •David Marecek[1], Julian Oberreiter[1], Andrew Nelson[2], and Stefan Kowarik[1] — [1]Physikalische und Theoretische Chemie, Universität Graz, Graz, 8010, Austria — [2]ANSTO, Locked Bag 2001, Kirrawee DC, NSW, 2232, Australia

We present an approach for analysis of real-time X-ray reflectivity (XRR) process data not just as a function of the reciprocal space vector q as is commonly done, but as a function of both q and time. We restrict the real-space structures extracted from the XRR curves to be solutions of a physics-informed growth model, and use state-of-the-art convolutional neural networks (CNNs) and differential evolution fitting to co-refine multiple time-dependent XRR curves *R(q,t)* of a thin film growth experiment. Thereby it becomes possible to correctly analyze XRR data with a fidelity corresponding to standard fits of individual XRR curves even if they are sparsely sampled with a 7-fold reduction of XRR datapoints, or if the data is noisy due to a 200-fold reduction in counting times. Our approach of using a CNN analysis and of including prior information through a kinetic model is not limited to growth studies, but can be easily extended to other kinetic X-ray or neutron reflectivity data to enable faster measurements with lower beam damage.

DS 1.4 Mon 10:15 H14

Scattergram analysis and filtering of differential phase contrast STEM images — •Julius Bürger[1,2], Maja Groll[1,2], Thomas Riedl[1,2], and Jörg K. N. Lindner[1,2] — [1]Nanostructuring, Nanoanalysis and Photonic Materials Group, Dept. of Physics, Paderborn University, Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn, Germany

Differential phase contrast (DPC) in scanning transmission electron microscopy allows the imaging and quantification of electric fields in solid specimen by measuring the transferred (first) momentum perpendicular to the optical axis imposed on the beam by the specimen's electrostatic potentials. Owing to the high-resolution capability of modern Cs-corrected transmission electron microscopes, electric fields and charge densities can be revealed with sub-atomic resolution. However, the requirements are very high, since the field distributions being measured by a position sensitive detector are drastically influenced by numerous factors, such as the lens aberrations, dynamic diffraction effects, noises, and the detector response function. We demonstrate how these influences can be readily detected in a DPC image using the so-called scattergram, which is a two-dimensional histogram of all transferred momenta, and particularly focus on the effect of noise and detector rotation by comparing DPC measurements and simulations for Si [110] performed with a segmented annular quadrant detector. In this regard, we introduce a novel method, the scattergram filtering, revealing the position of characteristic features in DPC images.

DS 1.5 Mon 10:30 H14

Contrast modes in transmission experiments using broad and focussed keV ion beams — •Svenja Lohmann[1,2], Gregor Hlawacek[1], Radek Holeňák[2], Nico Klingner[1], Daniel Primetzhofer[2], and Eduardo Serralta[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [3]Technische Universität Dresden, Germany

The helium ion microscope (HIM) is an instrument for high-resolution imaging, composition analysis, and materials modification at the nanoscale. Ion transmission experiments could further improve the analytical capabilities of this technique, and multiple contrast modes are possible. We explore the latter at keV ion energies using a HIM in a scanning transmission approach as well as a broad beam in combination with a time-of-flight (ToF) set-up. Both systems employ position-sensitive detectors allowing for analysis of angular distributions.

In the ToF-system, we find a strong trajectory-dependence of the measured specific energy loss attributed to charge-exchange events in close collisions [Phys. Rev. Lett. 124 (2020), 096601]. Channelling and blocking of transmitted ions allows for mapping of intensity as well as different energy loss moments [Ultramicroscopy 217 (2020), 113051]. In the HIM we demonstrate different contrasts, e.g., due to orientation of nanocrystals, channelling in single-crystalline membranes and material contrast for layered films [Beilstein J. Nanotechnol. 11 (2020), 1854].

DS 2: Focus Session: Innovative GaN-based High-power Devices: Growth, Characterization, Simulation, Application 1

Organizers:
Bernd Witzigmann, University Erlangen-Nürnberg
Frank Bertram, Magdeburg University

The transition to globally sustainable energy generation requires a further significant rise of sharing electrical energy. Power electronics is a key technology enabling efficient distribution, conversion, and use of these large amounts of electrical energy. Thanks to the advances in semiconductor materials with solid-state properties, power electronics research remains a focal point. The remarkable progress in wide-bandgap semiconductor materials such as Gallium Nitride (GaN) allows for power devices reaching switching speeds an order of magnitude above the state of the art, with significantly reduced ohmic and dynamic losses, and improved thermal properties. GaN-based devices and circuits therefore enable the design of highly compact power-electronic systems with highest efficiencies. Considerable energy savings are possible, e.g. with energy and vehicle technology alone, a previously unused potential of up to 35% can be exploited. This not only offers economic advantages, but also significantly reduces the CO_2 equivalents associated with the applications.

Time: Monday 9:30–11:15 Location: H17

Invited Talk DS 2.1 Mon 9:30 H17
GaN-based power converters enabling talktive power — •Marco Liserre — Kiel University, Kiel, Germany

GaN power semiconductors with their extremely fast switching characteristics enable not only electrical energy conversion which is almost free from switching losses but also to bridge for the first time two fields which have been developing separately for more than 70 years: energy and information transfer. This contribution will start from the physical characteristics of GaN power semiconductors to show what they allow in power conversion and how they can lead to realize power exchange which carries also information.

Invited Talk DS 2.2 Mon 10:00 H17
Energy-efficient power electronics based on Gallium Nitride — •Oliver Ambacher — Sustainable Systems Engineering (INATECH), Albert-Ludwigs-Universität, Freiburg

Around 40% of the energy converted worldwide by technical systems is already provided in the form of electricity. This share is expected to increase to around 60% in 2040. These enormous amounts of energy not only have to be generated in a way that conserves resources and the environment, but also distributed and used efficiently. The power electronics required for this is an *emerging field* of electrical engineering, which makes it possible to provide electrical energy optimally adapted for a wide variety of applications. These applications include the integration of renewable energy sources into the electrical supply network, drive technology for electromobility, the power supply for data centers or the high-frequency network for mobile communications. Using the example of the development and use of particularly energy-efficient gallium nitride-based power electronic circuits, the presentation will illustrate the high potential for saving energy that further optimization of semiconductor materials and microelectronic components offers and how sustainable electronic systems can be realized from them. Based on a basic understanding of the *atomic building blocks*, functional material properties are derived and presented for the design of novel power electronic devices and components. These GaN-based components are demonstrated for high performance amplifiers and voltage converters that are characterized by particularly energy-efficient operation.

DS 2.3 Mon 10:30 H17
Influence of space-charge region on luminescence in a lateral GaN superjunction — •Gordon Schmidt[1], Peter Veit[1], Frank Bertram[1], Jürgen Christen[1], Arne Debald[2], Michael Heuken[2,3], Thorsten Zweipfennig[2], Holger Kalisch[2], and Andrei Vescan[2] — [1]Otto-von-Guericke-University Magdeburg, Magdeburg, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]AIXTRON SE, Herzogenrath, Germany

The superjunction concept, based on charge compensation in the drift region by fully balanced n- and p-regions, is intended to break the tradeoff between breakdown voltage and on-resistance in GaN-based power devices.

In this study, a lateral GaN p-n^+ superjunction was investigated by scanning transmission electron microscope cathodoluminescence microscopy. The structure was grown on top of a GaN/sapphire template. After the growth of an AlGaN marker layer, the superjunction was epitaxially deposited composed of alternating 91 nm thick p-GaN with $5 \cdot 10^{18}$ cm^{-3} Mg doping and 23 nm thick n^+GaN with $1 \cdot 10^{19}$ Si doping. Finally, the structure was capped by a n^+GaN layer. To probe the space charge region of the superjunction, the luminescence evolution across the pn^+p junctions was investigated at T = 16 K. Donor-acceptor-pair recombination (DAP) is dominating the spectrum in the n-doped layers. In the near-band-edge region, bound exciton luminescence is observed in GaN:Mg. Both, excitons bound to an acceptor as well as to a donor exhibit reduced intensity in the space-charge region indicating exciton dissociation by the built-in electric field.

Invited Talk DS 2.4 Mon 10:45 H17
Potential of Aluminum Nitride for Vertical Power Electronics — •Andreas Waag[1,2], Klaas Strempel[1,2], Lukas Peters[1,2], Christoph Margenfeld[1,2], Samuel Faber[3], Friedhard Römer[3], and Bernd Witzigmann[3] — [1]Institute of Semiconductor Technology, Technische Universität Braunschweig, Hans-Sommer-Straße 66, 38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology (LENA), Technische Universität Braunschweig, Langer Kamp 6, 38106 Braunschweig, Germany — [3]Institute for Optoelectronics, Friedrich-Alexander Universität Erlangen-Nürnberg, Konrad-Zuse Str. 3/5, 91052 Erlangen, Germany

Owing to its excellent material properties, AlN is considered to be highly promising for power electronics. One of the main obstacles for AlN, however, is the poor availability of single crystal substrates. A particularly promising technique is the high temperature annealing (HTA) of sputtered AlN thin films on sapphire. AlN is one of the few compound semiconductors, which is curing its crystal lattice during HTA without thermal decomposition or evaporation if processed in a face-to-face configuration.

In addition to the material aspects, we discuss the design of AlN devices, supported by TCAD simulations, combining microscopic drift-diffusion currents with electron/hole continuity equations and the Poisson equation.

DS 3: 2D Materials 1 (joint session HL/CPP/DS)

Time: Monday 9:30–12:45 Location: H36

Invited Talk DS 3.1 Mon 9:30 H36

g-factors in van der Waals heterostructures: revealing signatures of interlayer coupling — •Paulo E. Faria Junior — University of Regensburg, Regensburg, Germany

The interplay of the spin and the orbital angular momenta of electrons in semiconductors governs the observed Zeeman splitting, often described by the effective g-factors. In the realm of 2D materials, transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of coupled spin and orbital degrees of freedom under external magnetic fields. In this talk, I will cover the basic physics behind the Zeeman splitting and effective g-factors, emphasizing the recent first-principles developments in monolayer TMDCs that nicely reproduce the available experimental data. These new theoretical insights demystify the valley-Zeeman physics in TMDCs and finally establish a connection to the vast existing knowledge in the area of III-V materials. Beyond monolayers, I will discuss TMDC-based van der Waals heterostructures, particularly MoSe2/WSe2 and WS2/graphene systems, in which the spin-valley physics and g-factors encode valuable information about the interlayer coupling.

DS 3.2 Mon 10:00 H36

Optical Properties of Encapsulated Transition-Metal Dichalcogenide Monolayers, Bilayers, and Heterostructures — •Manan Shah[1], Philip Klement[1], Sangam Chatterjee[1], Kyungnam Kang[2], Eui-Hyeok Yang[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany — [2]Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, NJ, 07030, USA

Van-der-Waals heterostructures (vdW-HSs) based on 2D-layered materials have received unrivaled attention among nanomaterials due to their promising optoelectronic properties induced by moiré potential landscapes; secondly, their strong light-matter interactions; and third, the promise of bandgap engineering capabilities. The optical properties of transition-metal dichalcogenides (TMDs) depend considerably on the substrate, stacking configuration, interface quality, and encapsulation. As more and more layered materials have come into the focus, the demand for a comprehensive understanding of their optical, optoelectronic, and vibronic properties is increasing drastically.

We focus on the discussion of photoluminescence and the Raman response of tungsten-based TMD monolayers and stacks thereof [1, 2], as well as encapsulated configurations. We further aim at unraveling structural alterations and emission properties by monitoring the temporal behavior in their responses. [1] Semiconductors 2019, 53, 2140. [2] Sci. Rep. 2022, 12, 6939.

DS 3.3 Mon 10:15 H36

Electrically Tunable Photoluminescence in Monolayer MoS_2 and graphene/MoS_2 Heterostructures — •Tarlan Hamzayev and Giancarlo Soavi — Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany

The optical response of monolayer (ML) transition metal dichalcogenides (TMDs) is dominated by the co-existence, even at room temperature, of excitons, bi-excitons, and trions.

The photoluminescence (PL) emission of these quasi-particles can be modulated via external knobs, such as doping, pressure and strain. In particular, the PL emission from the neutral exciton is greatly modulated during the crossover from the undoped to the highly doped regime [1]. In the latter case, PL emission is mainly suppressed due to the presence of trions, which have a fast non-radiative decay.

In this work, we study the gate dependence of the PL emission in encapsulated ML MoS_2 and ML graphene/MoS_2 heterostructures (HS). We show that in the HS region the PL emission mainly comes from neutral excitons even at large values of external gate voltage, thus confirming that graphene is an efficient filter for PL emission [2]. This work clarifies the interplay between charge transfer and PL filtering in graphene/TMD layered HS.

[1] Mak, K. F. et al. Nature materials 12, 207-211 (2013).

[2] Lorchat, E. et al. Nature Nanotechnology 15, 283-288 (2020).

15 min. break

DS 3.4 Mon 10:45 H36

Integration of Transferable Organic Semiconductor Nanosheets with 2D Materials for van der Waals Heterojunction Devices — •Sirri Batuhan Kalkan[1], Emad Najafidehaghani[2], Ziyang Gan[2], Fabian Alexander Christian Apfelbeck[1], Uwe Hübner[3], Antony George[2], Andrey Turchanin[2], and Bert Nickel[1] — [1]Faculty of Physics and CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 Munich, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, Lessingstr. 10, 07743, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745, Jena, Germany

Evaporation of organic semiconductors (OSC) on atomically thin transition metal dichalgonides (TMD) for van der Waals (vdW) heterojunctions is limited by obstructed growth of the organic small molecules on the TMD surface. For the realization of such vdW heterojunction devices, we have established a transfer technique that allows for wafer-scale fabrication of 50 nm OSC nanosheets on TMDs. A key feature of this transfer is the controlled release of the ultrathin OSC film from a water-soluble sacrificial film by a suited wetting geometry. We demonstrate functional and highly ordered OSC nanosheets on prefabricated electrodes and TMD monolayers. Devices fabricated this way include unipolar, ambipolar and anti-ambipolar field-effect transistors [1].

References: [1] Kalkan et al., Wafer scale synthesis of organic semiconductor nanosheets for van der Waals heterojunction devices, npj 2D Materials and Applications 5, 92 (2021)

DS 3.5 Mon 11:00 H36

Non-resonant and resonant low-frequency Raman scattering in twisted TMDC bilayers at millikelvin temperatures — •Hendrik Lambers[1], Nihit Saigal[1], Torsten Stiehm[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Twisted TMDC bilayers are subject of many current studies because they can host many body physics and correlated phases such as superconductors and Mott insulators.[1] The moiré potential evolving with a twist angle or lattice constant mismatch could also be exploited to simulate Mott-Hubbard physics. The interlayer coupling within the bilayer correlates with the interlayer breathing mode and the shear mode, which can be characterized by low frequency Raman spectroscopy.[2] We study TMDC heterobilayers of WSe2 and MoSe2 by resonant and non-resonant Raman spectroscopy at millikelvin temperatures. The shear mode is resonant with the exciton transitions in both monolayers and its lineshape and transition energy are modified due to coupling to the exciton continuum. In addition, several sharp and highly resonant modes are observed in the high frequency Raman spectrum. We acknowledge financial support via DFG WU 637/7-1 and SPP2244. [1] L. Sigl et al., Phys. Rev. Research 2, 042044(R) (2020) [2] J. Holler et al., Appl. Phys. Lett. 117, 013104 (2020)

DS 3.6 Mon 11:15 H36

Investigating Twist Angle Dependence of Exciton Resonances in WSe_2/$MoSe_2$ Heterostructures — •Chirag Palekar, Tobias Manthei, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

Artificially produced TMDC heterostructures (HS) realized by stacking two different TMDC monolayers (ML) are a new class of promising semiconducting heterostructures. Due to their type-II band alignment, TMDC HSs tend to host the spatially indirect interlayer excitons (IX) where electrons and holes are located in conduction and valence bands, respectively, of the different layers. Here we study the twist angle dependence of IX resonances employing micro-photoluminescence excitation (PLE) measurements on twisted WSe_2/$MoSe_2$ heterobilayer. PLE measurements reveal anti-correlation between linewidth and emission energy of IX. Resonant excitation at intralayer exciton energies of constituent ML yields high emission intensity of the IX with linewidth narrowing above 10 meV. We measure a drastic reduction in PL emission from IX for twist angles in the range of 10°- 50° due to large inter-

layer separation. Moreover, we show a noticeable IX exciton resonance separation which increases as function of twist angle i.e. from 0° (67 meV) to 24° (96 meV) along with observable red shift in IX emission energy. This fundamental study of excitons resonances deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

DS 3.7 Mon 11:30 H36

Counterintuitive electric-field dependence of weak antilocalization in a bilayer graphene/WSe_2 heterostructure — Julia Amann[1], Tobias Völkl[1], Tobias Rockinger[1], Denis Kochan[2], Kenji Watanabe[3], Takashi Taniguchi[3], Jaroslav Fabian[2], Dieter Weiss[1], and •Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

Heterostructures of bilayer graphene (BLG) and transition metal dichalcogenides (TMDC) were recently proposed as a means of generating a gate-tunable, proximity-induced spin-orbit coupling (SOC) in graphene. Total SOC splitting of the band structure increases monotonically with the out-of-plane electric field, as confirmed by recent charge transport experiments. To elucidate the spin relaxation caused by SOC, weak antilocalization (WAL) experiments are frequently employed. Contrary to the naïve expectation of a monotonic increase of the WAL effect strength with electric field D, we observe a maximum of WAL visibility around $D = 0$. This counterintuitive behaviour originates in the intricate dependence of WAL in graphene on two different spin lifetimes τ_{sym} and τ_{asy}, which are due to spin relaxation caused by the valley-Zeeman and Rashba terms, respectively. Our calculations, based on modeling spin precession by an 8×8 Hamiltonian of BLG with one-sided TMDC show the same non-monotonic dependence on D as the experimental data.

15 min. break

DS 3.8 Mon 12:00 H36

Millikelvin Spectroscopy on Degenerate Exciton Ensembles in van der Waals Bilayers — •Nihit Saigal[1], Torsten Stiehm[1], Hendrik Lambers[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Homo- and hetero-bilayers of transition metal dichalcogenides host a rich variety of interlayer exciton (IX) species where the electrons and holes reside in different monolayers. [1] This leads to enhanced lifetimes of IXs and also imparts them with a permanent dipole moment. [1,2] Such IXs provide an ideal platform for exploring many body physics such as dipole-dipole interactions and Bose-Einstein condensation. [2] We have investigated IXs in a heterobilayer of MoSe2 and WSe2 encapsulated in hBN, using temperature, laser power and time dependent photoluminescence (PL) spectroscopy down to millikelvin temperatures. At lowest temperatures and exciton densities, we observe a single low energy peak in the IX PL spectrum which has been attributed to be a signature of degenerate exciton gas. [2] We observe an unexpected nearly excitation power-independent IX energies at lowest temperatures (10 mK to ~10K) that converts into the well-known dipolar blue-shift at elevated temperatures. We acknowledge financial support by DFG via WU 637/4-2 and No. HO 3324/9-2 and SPP2244.

[1] B. Miller et al., Nano Lett. 17, 5229 (2017). [2] L. Sigl et al., Phys. Rev. Research 2, 042044 (R) (2020).

DS 3.9 Mon 12:15 H36

Infrared photocurrent in transition-metal dichalcogenide heterostructures — Jeong Woo Han[1], Peize Han[2], Yijing Liu[2], Paola Barbara[2], Thomas E. Murphy[3], and •Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Georgetown University, Department of Physics, Washington, 20057 DC, USA — [3]University of Maryland, Institute for Research in Electronics and Applied Physics, College Park, 20740 MD, USA

Heterostructures of transition metal dichalcogenites (TMDCs) have characteristic optical properties like the interlayer excitons due to the band offset between two adjacent TMDC layers. Such heterostructures are promising candidates for photodetectors with higher efficiencies compared to a single TMDC layer, furthermore, the interlayer excitation enables photocurrents at photon energies below the direct bandgap of each of the layers. Here we present measurements on a MoS_2/WS_2 heterostructure at photon energies of around 800 meV, which is significantly below the interlayer exciton. The cross-shaped structure of our samples allows measurements of the heterostructure as well as each individual layer. While at high photon energies photocurrents are observed in each of the layers, the low photon energy only leads to a photocurrent when the heterostructure is illuminated. We interpret this effect to be caused by intraband absorption and subsequent interlayer tunneling.

DS 3.10 Mon 12:30 H36

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and metal supercrystals — •Lara Greten, Robert Salzwedel, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of transition metal dichalcogenides (TMDC) are direct semiconductors that exhibit tightly bound excitons with uniquely large optical amplitudes. Thus, they are promising for optoelectronic applications and a prime example to investigate excitonic effects.

Complementary, plasmonic supercrystals, that are arrays of metal nanoparticles, support collective plasmon modes. They facilitate an impressive amplification of the electric near-field which allows to tailor electric fields on the nano-scale.

In the presented work, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a single metal nano-particle or a two-dimensional supercrystal. For this purpose, we develop a Maxwell-Bloch theory where the excitons are described within the Heisenberg equation of motion framework and the metal nano-particles are treated as coupled dipoles in Mie theory.

Our studies reveal new "plexcitonic" eigenstates of the hybrid system. Furthermore, we are able to compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling featuring a Rabi splitting of tens of meV.

DS 4: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 2

Time: Monday 11:00–11:45 Location: H14

DS 4.1 Mon 11:00 H14

Scaling and confinement in ultrathin chalcogenide films as exemplified by GeTe — •Peter Kerres — 1st Institute of Physics "new Materials", RWTH Aachen University, 52066 Aachen, Germany

Chalcogenides such as GeTe, PbTe, Sb2Te3, and Bi2Se3 are characterized by an unconventional combination of properties enabling a plethora of applications ranging from thermo-electrics to phase change materials, topological insulators and photonic switches. Chalcogenides possess pronounced optical absorption, relatively low effective masses, reasonably high electron mobilities, soft bonds, large bond polarizabilities and low thermal conductivities. These remarkable characteristics are linked to an unconventional bonding mechanism characterized by a competition between electron delocalization and electron localization. Confinement, i.e. the reduction of the sample dimension as realized in thin films should alter this competition and modify chemical bonds and the resulting properties. Here, we demonstrate for crystalline films of GeTe pronounced changes of optical and vibrational properties, while amorphous films of GeTe show no similar thickness dependence. For crystalline films, this thickness dependence persists up to remarkably large thicknesses of 40 nm. x-ray diffraction and accompanying simulations employing density functional theory relate these changes to thickness dependent structural (Peierls) distortions, due to an increased electron localization between adjacent atoms upon reducing the film thickness. We expect a thickness dependence and

hence potential to modify film properties for all chalcogenide films with a similar bonding mechanism .

DS 4.2 Mon 11:15 H14

Solid-state microstructural evolution and dewetting of Co_xCu_{100-x} thin films — •Farnaz Farzam[1], Bárbara Bellón[1], Matteo Ghidelli[1,2], María Jazmin Duarte Correa[1], Dominique Chatain[3], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]LSPM, CNRS, Université Sorbonne Paris Nord, Villetaneuse, France — [3]Aix-Marseille Univ, CNRS, CINaM, Marseille, France

Metallic thin films can undergo severe microstructural and morphological evolution, while maintaining their solid state at high temperatures below their melting point(T_M). These structural changes such as hillock formation and texture evolution can be followed by solid-state dewetting(SSD) in which capillary forces finally break up the film into isolated particles. Here, we investigate the microstructural evolution of Co_xCu_{100-x} thin films with x equal to 15, 38 and 75 at.%. Films were deposited on (0001) sapphire and annealed below their T_M. Subsequently, characterization has been carried out using scanning and transmission electron microscopy(SEM, TEM), and X-ray diffraction(XRD). Upon annealing, Cu-rich hillocks form in all three compositions prior to voids at which dewetting initiates. The onset temperature of the formation of these hillocks depends on the composition of the film. Moreover, a phase separation of FCC Co and FCC Cu is observed. Finally, we show an orientation relationship of Cu (FCC) and Co (FCC)-rich isolated particles with sapphire: $Cu/Co(111) \pm [1\bar{1}0] \parallel Al_2O_3(0001)[10\bar{1}0]$.

DS 4.3 Mon 11:30 H14

Analysis of 3D check board pattern formation in NiCoMnAl shape memory alloys with alternating austenitic and martensitic layers — •Dario Stierl, Andreas Becker, Laila Bondzio, Tapas Samanta, Inga Ennen, and Andreas Hütten — Center for Thin Films and Physics of Nanostructures, Physics Department, Bielefeld University, 33615 Bielefeld, Germany

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 XRD and temperature dependent magnetization measurements.

DS 5: Organic Thin Films, Organic-Inorganic Interfaces

Time: Monday 11:30–13:00 Location: H17

DS 5.1 Mon 11:30 H17

RuTPP thin films: morphology, dimerization and CO adsorption — •Jakob Hauns[1], Johannes Seibel[1], Artur Böttcher[1], Lukas Gerhard[2], Wulf Wulfhekel[2], and Manfred Kappes[1] — [1]Institute of Physical Chemistry, KIT, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, KIT, 76344, Eggenstein-Leopoldshafen, Germany

Thin RuTPP-2H films were grown on HOPG under UHV conditions by applying the Low Energy Cluster Beam Deposition method, LECBD [1]. We used the mass-selected (RuTPP-2H)+ beam resulting from electron impact induced ionization and fragmentation of the effusive flux of RuTPP molecules. The morphology of the films grown here were systematically studied by means of STM, UPS, XPS and desorption spectroscopy. The temperature programmed desorption (TPD) spectra, taken for sub- and multilayers enable to determine the binding energies explaining the unique stability of the films. In particular this analysis revealed the thermally activated formation of stable desorbable dimers for layers thicker than one monolayer. By combining STM and UPS we found spectral markers for the monomers and dimers deposited on HOPG. XPS/UPS based study of the CO adsorption on RuTPP-2H submonolayers revealed pronounced modifications of the valence band. These findings are supported by extensive DFT calculations which enable to identify the major CO-(RuTPP-2H) binding sites.

[1] J. Weippert, et al., J. Phys. Chem. C 2018, 122, 28588*28600

DS 5.2 Mon 11:45 H17

Low-Temperature Atomic Layer Deposition of Al_2O_3 Thin Films on Spin-Coated Carbon Nanomembranes — •Jan Biedinger, Natalie Frese, Raphael Dalpke, Bernhard Kaltschmidt, Martin Wortmann, Andreas Hütten, Armin Gölzhäuser, and Günter Reiss — Bielefeld University, Germany

Carbon nanomembranes are stable, carbon-based 2D sheets that have been investigated in recent years due to their wide range of potential applications, in nanofiltration, nanoelectromechanical systems, microelectronics or energy storage [1]. Atomic layer deposition relies on alternating self-limiting gas-surface reactions, resulting in smooth, conformal and defect-free coatings with precise thickness control [2]. In the presented work, carbon nanomembranes were coated with aluminum oxide (Al_2O_3) via a thermal atomic layer deposition process at a substrate temperature of 60°C including the reactants trimethylaluminum and water. Structural and compositional investigations of these bilayer systems by atomic force, helium ion and transmission electron microscopy as well as depth profile X-ray photoelectron spectroscopy and energy dispersive X-ray analysis, respectively, reveal a homogeneous and conformal coating of the entire sample, resulting in effective surface modification. In addition, gas permeation measurements were carried out to explore potential applications of such hybrid membranes, demonstrating atomic layer deposition offers a simple way of tuning carbon nanomembranes.

[1] A. Turchanin and A. Gölzhäuser, Adv. Mater. 28, 6075 (2016)
[2] S. M. George, Chem. Rev. 110, 111 (2010)

DS 5.3 Mon 12:00 H17

Contact Primers: A new Approach to Reducing Contact Resistance in Organic Field-Effect Transistors — •Yurii Radiev and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35037 Marburg, Germany

Methods to reduce contact resistance have long been of interest to researchers that aim to improve performance of organic electronic devices. Caused by the injection barrier at the metal-organic semiconductor interface, contact resistance was shown to be one of the main obstacles on the way to producing high-frequency organic field-effect transistors (OFETs), limiting the switching frequency of such transistors to well below gigahertz range [1]. In this work we report on the contact primer method [2] – a method that allows selective modification of the work function of the electrodes in a bottom gate-bottom contact OFET structure. The modified work function reduces the charge carrier injection barrier and improves the morphology of the subsequently deposited thin film on top. We demonstrate this effect for both p- and n-type OFETs by employing various organic contact primer materials to increase and reduce the work function of gold electrodes, respectively. Combining this device-oriented approach with a rigorous investigation of the employed material systems on model substrates, we are able to achieve deeper understanding of the phenomena that lead to a reduced contact resistance [3].

[1] U. Zschieschang, et al., Adv. Func. Mater. 30, 1903812 (2020).
[2] F. Widdascheck, et al., Adv. Funct. Mater. 29, 1808385 (2019).
[3] Y. Radiev, et al., Org. Electron. 89, 106030 (2021).

DS 5.4 Mon 12:15 H17

Patterned Growth of Organic Semiconductor Films by Electron Irradiation Induced F-Centers on Alkali Halide Substrates — •Darius Günder[1], Valentin Diez-Cabanes[2], Andrea Huttner[1], Tobias Breuer[1], Vincent Lemaur[2], Jerome Cornil[2], and Gregor Witte[1] — [1]Molekulare Festkörperphysik, Philipps-Universität Marburg — [2]Laboratory for Chemistry of Novel Materials,

University of Mons

In this study, a new approach is introduced to control structural properties of organic films. Combining AFM, SEM and XRD we demonstrate that electron irradiation induced F-centers (halide vacancies) on KCl(100) surfaces strongly influence the molecular orientation and epitaxial alignment of dinaphtothienothiophene (DNTT) thin films. Due to electrostatic interactions between F-centers and interfacial DNTT molecules, as validated by DFT calculations, DNTT molecules adopt a recumbent molecular orientation and form elongated fibers instead of hexagonally shaped island with upright molecular orientation present on pristine KCl. Interestingly, both morphologies exhibit epitaxial alignments that are understood by higher-order commensurabilities. By inducing F-centers only at defined surface regions, this F-center controlled growth is utilized to achieve laterally patterned DNTT films that are even transferable to other substrates by a wet transfer process.

DS 5.5 Mon 12:30 H17

The Role of Molecular Packing in Strongly Coupled Metal-Organic Hybrid Structures — •Maximilian Rödel[1], Polina Lisinetskaya[2], Maximilian Rudloff[1], Thomas Stark[3], Jochen Manara[3], Roland Mitric[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institut für Physikalische und Theoretische Chemie, University of Würzburg, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg

The coupling between excited states in fluorinated zinc-phthalocyanine thin films (F_nZnPc, with n = 0,4,8,16) and surface plasmons in gold layers underneath enables unique insights in the resulting exciton-plasmon polariton coupling phenoma and their energetics. In particular, the increase of the molecular van der Waals radii by the degree of fluorination offers an additional degree of freedom to analyze the role of molecular orientation and aggregation on the resulting dispersion curves. As such, we were able to identify up to four anticrossings in the layered Au/F_nZnPc samples which can be attributed to: 1) a co-existing $F_{16}ZnPc$ β-polymorph, 2) monomers, preferentially located at the metal interface, and 3) aggregated α-phase regions located within the F_nZnPc films. While energy and splitting of the monomer-related anticrossing are determined by the average tilting and the close proximity to the metal surface, the coupling associated with the aggregate can be consistently described by a change in F_nZnPc dipole density. Supported by structural data and TDDFT calculations in combinations with a Jaynes-Cummings model, Au/F_nZnPc bilayers proof to be a versatile platform to study the primary light-matter interactions.

DS 5.6 Mon 12:45 H17

Strong Quenching of Dye Fluorescence in Perylene Orange/TMDC Hybrid Structures — •Tim Völzer, Alina Schubert, Erik von der Oelsnitz, Ingo Barke, Sylvia Speller, Tobias Korn, and Stefan Lochbrunner — Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23, 18059 Rostock

While monolayer transition metal dichalcogenides (1L-TMDCs) have emerged as 2D semiconductors with multiple applications in optoelectronics, their combination with dye molecules to form promising hybrid structures, since they should allow charge transfer after optical excitation as required for photodetectors or solar cells. Here, we discuss the preparation of such systems, i.e. the deposition of perylene orange (PO) onto substrates by means of spin coating, stamping, and thermal vapor deposition (TVD) and compare these methods regarding the quality of the dye layer and practicability of the process. For TVD-fabricated 1L-TMDC/PO hybrid structures, we observe a drastic quenching of the dye fluorescence in terms of both intensity and lifetime reduction for all used TMDCs compared to hBN/PO references. This quenching is attributed to electron or hole transfer depending on the energy levels of the molecule and the specific TMDC, respectively.

DS 6: Focus Session: Innovative GaN-based High-power Devices: Growth, Characterization, Simulation, Application 2

Organizers:
Bernd Witzigmann, University Erlangen-Nürnberg
Frank Bertram, Magdeburg University

Synopsis (see part I)

Time: Monday 15:00–16:45 Location: H17

Invited Talk DS 6.1 Mon 15:00 H17

Novel high power device structures: Enabling compact and integrated power ICs — •Elison Matioli — EPFL, Lausanne, Switzerland

This talk will discuss new technologies to drastically reduce the sheet resistance in these semiconductors. Combined with a judicious design of the electric field distribution, based on nanostructures, this approach enables to concurrently reduce the on-resistance and increase the breakdown voltage of power devices, leading to figures of merit far beyond the state-of-the-art. To manage the large heat fluxes in power devices, I will present new technologies based on integrated microfluidic cooling inside the device. By co-designing microfluidics and electronics within the same semiconductor substrate, a monolithically integrated manifold microchannel cooling structure was produced with efficiency beyond what is currently available. Our results show that heat fluxes exceeding 1.7 kW/cm2 could be extracted using only 0.57 W/cm2 of pumping power. The proposed cooling technology should enable further miniaturization of electronics, and greatly reduce the energy consumption in cooling of electronics. Furthermore, by removing the need for large external heat sinks, this approach enables the realization of very compact power converters integrated on a single chip.

Invited Talk DS 6.2 Mon 15:30 H17

Ab-initio investigations of V-pits and nanopipes in GaN — •Liverios Lymperakis[1,2], Su-Hyun Yoo[2], and Jörg Neugebauer[2] — [1]Department of Physics, University of Crete, Heraklion, Greece — [2]Computational Materials Design Department, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Dislocations in nitrides constitute a long-standing and controversial topic. Nevertheless, screw dislocations in GaN have recently attracted considerable interest due to their potential effect on power electronic devices' performance. An intriguing feature of these dislocations is that they trigger the formation of V-pits and nanopipes in GaN. However, a full understanding of their origin, size, and shape is still lacking. The nucleation and properties of these defects are governed by the complex interplay between dislocation's strain and core energies, surface energies, and oversaturation. In the present work, we combine density functional theory calculations with elasticity theory and we shed light on the aforementioned interplay. Based on these calculations we derive phase diagrams that describe the equilibrium size and shape of V-pits and nanopipes as a function of the ambient growth conditions, i.e., the Ga and H chemical potentials as well as the oversaturation. Our calculations indicate that under H-rich conditions, V-pits and nanopipes can spontaneously form due to the preferential decoration of the bounding surfaces by hydrogen. Based on these results we will further discuss their electronic properties as well as their potential to preferentially accommodate impurities/dopants.

DS 6.3 Mon 16:00 H17

Metal micro-contacts deposited by focused electron and ion beam: impact on electrical properties — •Konstantin Wein, Gordon Schmidt, Frank Bertram, Silke Petzold, Peter Veit, Christoph Berger, André Strittmatter, and Jürgen Christen — Otto-von-Guericke-University Magdeburg, Magdeburg, Germany

In this study, we want to concentrate on the local deposition of platinum and tungsten as metal micro-contacts by electron- as well as ion-beam in a focused ion beam microscope (FIB). We are using a

Thermo Fisher Scientific Scios 2 HighVac dual-beam with liquid gallium ion source. Either the focused electron beam or the ion beam are used to crack the precursor molecule bonds and induce the complex metal deposition process.
For the investigation of the electrical properties Pt/W stripes were deposited between macroscopic lithographic Au pads on top of insulating SiO_2/Si template. Parameters like Ga- and e-beam current, acceleration voltage, dwell time and pixel overlap were systematically investigated and optimized with regard to best electrical properties. The trade-off between efficient incorporation of conductive material and sputtering has to be determined. We observe almost insulating properties for layers deposited by electron beam radiation. On the other hand, the ion beam induced deposition layers behave ohmic and exhibit electrical conductivity up to $4.6\frac{10^5}{\Omega * m}$ for tungsten.

Invited Talk DS 6.4 Mon 16:15 H17

Lateral and Vertical β-Ga_2O_3 Power Transistors for High-Voltage Applications — •Kornelius Tetzner[1], Michael Klupsch[1], Karina Ickert[1], Ralph-Stephan Unger[1], Zbigniew Galazka[2], Ta-Shun Chou[2], Saud Bin Anooz[2], Andreas Popp[2], Joachim Würfl[1], and Oliver Hilt[1] — [1]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik (FBH), Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Straße 2, 12489 Berlin, Germany

Beta gallium oxide (β-Ga_2O_3) with its ultra-wide bandgap of 4.8 eV has emerged as a promising semiconducting material for the fabrication of next-generation power electronic devices. The estimated dielectric strength of 8 MV/cm in combination with the expected Baliga's figure of merit are promising indicators to pave the way for the realization of power devices with even higher breakdown voltages and efficiencies than their SiC and GaN counterparts. This presentation will give an overview on the current status of lateral and vertical β-Ga_2O_3 power transistor devices with a special emphasis on results obtained at FBH and IKZ. For both cases different concepts for bulk crystal growth, epitaxial layer structures and device designs suitable for reaching the targeted performance will be discussed especially in terms of breakdown voltage and channel current density. In this regard, certain material and device related challenges are identified which need to be addressed perspectively in order to overcome current breakdown limitations.

DS 7: 2D Materials 2 (joint session HL/CPP/DS)

Time: Monday 15:00–18:30 Location: H36

DS 7.1 Mon 15:00 H36

On-demand light emission from helium ion induced defects in atomically thin WS_2 — •Nina Pettinger, Ana Micevic, Alexander Hötger, Christoph Kastl, and Alexander Holleitner — TU Munich, Germany

Optically active defects created with a helium ion microscope (HIM) propose the possibility for structuring and tailoring quantum emitters on an atomistic scale [1]. We introduce the generation of positioned defects in encapsulated monolayer WS_2 with a HIM. The HIM induced defects exhibit sharp photoluminescence emission in the energy range of 1.55 to 1.79 eV.

[1] J. Klein and L. Sigl et al., ACS Photonics 8, 669 (2021).

DS 7.2 Mon 15:15 H36

Concept of an all-optical THz near-field microscope for flakes of 2D materials — •Ahmad-Reza Etemadi, Sebastian Matschy, Ahana Bhattacharya, and Martin Mittendorff — Department of physics, University of Duisburg-Essen, 47057 Duisburg, Germany

While THz spectroscopy is an excellent tool to investigate the free charge carriers in many semiconducting materials, the long-wavelength is an inherent feature linked to a large spot size in the millimeter range, and thus large samples are required. Small flakes of two-dimensional materials exfoliated from bulk crystals are usually much smaller than the spot size of a conventional THz spectrometer. The direct detection of the THz signal in the vicinity of the flake gains the phase and amplitude information with a higher spatial resolution. This is accessible by placing the sample directly on top of an electro-optic crystal. Sampling the THz field at the flake position gives access to the complex conductivity and thus the carrier density as well as the carrier mobility. A frequency-doubled fiber laser with a pulse duration of about 80 fs at 780 nm is exploited to generate and sample the THz field. GaSe, and ZnTe are employed as electro-optic crystals. Here we present the current state of the near-field microscope and the first measurements of the spatial resolution. The experimental results are accompanied by rigorous modeling of the THz propagation within the electro-optic crystal.

DS 7.3 Mon 15:30 H36

Ab initio description of valley-selective circular dichroism — •Maximilian Schebek[1], Yiming Pan[2], Cecilia Vona[1], Claudia Draxl[1], and Fabio Caruso[2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

By enabling control of valley degrees of freedom, valley-selective circular dichroism (VSCD) has become a key concept in valleytronics. In this work, we present an *ab initio* many-body theory of VSCD based on the Bethe-Salpeter equation. Our approach provides a new route to accurately predict the degree of valley polarization upon absorption of circularly polarized light. With the example of monolayer transition-metal dichalcogenides, we further show that valley excitons - bound electron-hole pairs formed at either the K or $\overline{\text{K}}$ valley upon absorption of circularly-polarized light - are chiral quasiparticles characterized by a finite orbital angular momentum (OAM). Beside governing the interaction with circularly polarized light, the OAM results in a finite magnetization of excitons, which in turn provides a route for the interaction of excitons with external magnetic fields and other spin-orbital degrees of freedom.

DS 7.4 Mon 15:45 H36

Dark and bright exciton dynamics probed by time-resolved photoluminescence in hBN-encapsulated $MoWSe_2$ monolayers — •Julian Schröer[1,3], Joanna Kutrowska-Girzycka[2], Leszek Bryja[2], Joanna Jadczak[2], and Jörg Debus[1] — [1]TU Dortmund, Experimentelle Physik 2, AG Debus — [2]Wroclaw University of Science and Technology, Department of Experimental Physics — [3]Universität Rostock, Institut für Physik, AG Korn: Zweidimensionale Kristalle und Heterostrukturen

Semiconducting monolayers of ternary $MoWSe_2$ alloys combine the unique properties of the binary transition metal dichalcogenide (TMDC) materials $MoSe_2$ and WSe_2. The alloying leads to, for example, brightening of the momentum- and spin-forbidden dark exciton states. Detailed studies on the dynamics of these brightened dark states are missing. We report on the exciton and trion formation lying in the 1-3 ps range, while the decay time approaches hundreds picoseconds. Additionally, strong dependences on the temperature and exciting laser light polarization are observed. In time-resolved and stationary photoluminescence measurements, we reveal the impact of the crystal disorder potential on the exciton properties. The polarization dynamics of the exciton and trion photoluminescence indicate possible contributions from chiral phonons as well as electrons and holes from different valleys of the Brillouin zone. Our work is a further step towards a deeper understanding of the dynamics of dark excitons in TMDC materials.

15 min. break

DS 7.5 Mon 16:15 H36

Signatures of a degenerate many-body state of interlayer excitons in a van der Waals heterostack — •Johannes Figueiredo[1], Lukas Sigl[1], Florian Sigger[1], Jonas Kiemle[1], Mirco Troue[1], Ursula Wurstbauer[2], and Alexander Holleitner[1] — [1]Walter-Schottky-Institut, Technical University of Munich — [2]Institute of Physics, Westfälische Wilhelms-Universität Münster

In atomistic van der Waals heterostacks of transition metal dichalcogenides, the reduced dimensionality and changing dielectric environement leads to the formation of stronlgy bound excitons. Optically generated interlayer excitons exhibit an additional spatial separation

of the electron-hole pair with a reduced overlap of the electrons' and holes' wave-functions, evidenced through their long lifetimes. These long-lived, photogenerated composite bosons yield several signatures of a quantum degenerate many-body system at cryogenic temperatures. The emergence of this state is in accordance with theoretical predictions of a critical condensation temperature above 10K. We present new insights into the phase-diagram of such interlayer exciton ensembles. [1]

[1] L. Sigl *et al.*, Phys. Rev. Research 2, 042044(R) (2020)

DS 7.6 Mon 16:30 H36

exciton species in highly doped WS_2 monolayers — DAVID TIEDE, •HOSSEIN OSTOVAR, HENDRIK LAMBERS, NIHIT SAIGAL, and URSULA WURSTBAUER — Institute of Physics, University of Münster, Münster, Germany

Semiconducting two-dimensional transition metal dichalcogenides such as WS_2 excel due to their exciton dominated light-matter interaction even at room temperature (RT) that is highly tunable by external stimuli such as doping, light excitation, dielectric environment, or strain [1]. In this work, an optimized field effect structure utilizing a polymer electrolyte top gate electrode is employed to study the evolution of the optical response in monolayer WS_2 at RT in dependence of doping by means of photoluminescence and spectroscopic imaging ellipsometry measurements. The huge geometrical gate capacitance enables capacitance spectroscopy of the conduction band as well as valence band edge yielding a gap energy of 2.6eV in agreement with the determination from the exciton Rydberg series. The gate allows the injection of large electron and hole densities exceeding $10^{14} cm^{-2}$, sufficient to enable the exciton Mott transition. The obtained doping dependent emission and absorption spectra also facilitate the identification of phonon activated, neutral and charged exciton species as well as dressed excitons in a fermi sea. We acknowledge financial support via DFG WU 637/7-1 and SPP2244. [1] U. Wurstbauer et al. J. Phys. D: Appl. Phys. 50, 173001 (2017).

DS 7.7 Mon 16:45 H36

Pump probe signatures of interlayer excitons in TMDC heterostructures — •HENRY MITTENZWEY, MANUEL KATZER, ANDREAS KNORR, and MALTE SELIG — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

TMDC heterobilayers are promising candidates for novel optoelectronic applications, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different layers. The relaxation dynamics of these interlayer excitons and their interplay with intralayer excitons are still under investigation.

Here, we present a microscopic description for the phonon and tunneling induced formation and relaxation of intra- and interlayer excitons in a $MoSe_2/WSe_2$ stack. Based on the microscopic dynamics we calculate the pump probe signal for intra- and interlayer transition and their population dynamics including hot exciton bottleneck effects.

DS 7.8 Mon 17:00 H36

Angle- and polarization-resolved luminescence from suspended and hBN encapsulated $MoSe_2$ monolayers — •BO HAN[1], SVEN STEPHAN[1], JOSHUA J.P. THOMPSON[2], MARTIN ESMANN[1], CARLOS ANTÓN-SOLANAS[1], HANGYONG SHAN[1], SAMUEL BREM[3], CHRISTOPH LIENAU[1], KENJI WATANABE[4], TAKASHI TANIGUCHI[4], MARTIN SILIES[1], ERMIN MALIC[2,3], and CHRISTIAN SCHNEIDER[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Philipps Universität, Marburg, Germany. — [3]Chalmers University of Technology, Gothenburg, Sweden. — [4]National Institute for Materials Science, Tsukuba, Japan.

We apply combined angle- and polarization-resolved spectroscopy to explore the interplay of excitonic physics and phenomena arising from the commonly utilized encapsulation on the optical properties of atomically thin transition metal dichalcogenides. In our study, we probe $MoSe_2$ monolayers which are prepared in both a suspended and an encapsulated manner. We show that the hBN encapsulation significantly enhances the linear polarization of exciton PL at large emission angles. This degree of linear polarization of excitons can increase up to 17 % in the hBN encapsulated samples. As confirmed by finite-difference time-domain simulations, it can be directly connected to the optical anisotropy of the hBN layers. In comparison, the linear polarization at finite exciton momenta is significantly reduced in suspended $MoSe_2$ monolayer, and only becomes notable at cryogenic conditions. This phenomenon strongly suggest that the effect is rooted in the k-dependent anisotropic exchange coupling inherent in 2D excitons.

15 min. break

DS 7.9 Mon 17:30 H36

Photonic and Phononic Couplings in Hybrid High-Q Nanocavities with Encapsulated MoS2 Monolayer — •CHENJIANG QIAN[1], VIVIANA VILLAFAÑE[1], PEDRO SOUBELET[1], ALEXANDER HÖTGER[1], TAKASHI TANIGUCHI[2], KENJI WATANABE[2], NATHAN WILSON[1], ANDREAS STIER[1], ALEXANDER HOLLEITNER[1], and JONATHAN FINLEY[1] — [1]Walter Schottky Institut and Physik Department, Am Coulombwall 4, 85748 Garching, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Monolayer TMDs are ideal active materials for solid-state cQED. However, the direct cou-pling of TMDs to 0D nanocavities whilst preserving pristine excitonic properties and large cavi-ty-TMD overlap remains a challenge. Most commonly, non-encapsulated TMDs are stacked on top of prefabricated photonic structures using pick-and-place assembly. In this case, environ-mental disorders strongly perturb the excitonic properties. Whilst disorder can be mitigated by full hBN encapsulation, this approach moves the TMD away from the cavity field, thereby, trad-ing spatial coupling for homogeneous linewidth. Here, we integrate hBN/MoS2/hBN heterostruc-tures to Si3N4 nanobeams as hybrid nanocavities. Our approach solves the trade-off problem by making the unpatterned heterostructure a functional part of the cavity field. Therefore, the pris-tine excitonic quality, high cavity mode Q-factor > 10000, and the strong cavity-MoS2 overlap are achieved simultaneously. We study the coupling of MoS2 excitons to the cavity optical and vibrational modes using PL and Raman spectroscopy, and novel coupling phenomena are ob-served based.

DS 7.10 Mon 17:45 H36

Terahertz free carrier absorption to modulate the optical properties of nanometer-thick van der Waals semiconductors — •TOMMASO VENANZI[1,2], MALTE SELIG[3], ALEXEJ PASHKIN[2], STEPHAN WINNERL[2], MANUEL KATZER[3], HIMANI ARORA[2], ARTUR ERBE[2], AMALIA PATANE[4], ZAKHAR R. KUDRYNSKYI[4], ZAKHAR D. KOVALYUK[5], LEONETTA BALDASSARRE[1], ANDREAS KNORR[3], MANFRED HELM[2], and HARALD SCHNEIDER[2] — [1]Sapienza University of Rome, 00185 Rome, Italy — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Technical University Berlin, 10623 Berlin, Germany — [4]University of Nottingham, Nottingham NG7 2RD, UK — [5]The National Academy of Sciences of Ukraine, 58001 Chernivtsi, Ukraine

Free carriers in doped semiconductors absorb terahertz radiation when the frequency of the electromagnetic field is lower or comparable to the plasma frequency of the system. This phenomenon can be used to manipulate the optical response of the material. We present here the results of two different experiments performed at the infrared free-electron laser FELBE on atomically-thin van der Waals semiconductors. In MoSe2 monolayers, we observe a terahertz-induced redshift of the trion resonance. Terahertz absorption induces an average high momentum to the carriers and this momentum gets transferred during the trion formation, resulting in a net redshift in the absorption. In few-layer InSe, the terahertz pulses induce a transient quenching of the photoluminescence emission. In both cases, a microscopic study of the hot carrier distribution cooling is also presented.

DS 7.11 Mon 18:00 H36

Theory of Exciton-Phonon Interaction for Stationary State Experiments in Atomically Thin Semiconductors — •MANUEL KATZER, ANDREAS KNORR, and MALTE SELIG — Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Atomically thin semiconductors exhibit tightly bound electron hole pairs which stimulated exciton research in recent years [1]. While typical experimental techniques include the cw excitation of the material, only few is known theoretically about the related exciton dynamics and the formation of non-equilibrium steady states. Based on excitonic Boltzmann scattering equations, we demonstrate that the formation of such stationary states is also accompanied with the formation of phonon replica in the photoluminescence excitation spectrum [2], in agreement with available experiments [3]. So far, many studies focused on the understanding of exciton dynamics in the limit of weak excitation. Above this limit, we find both bosonic but also fermionic contributions to the thermalization, due to the co-bosonic nature of

excitons. Based on a Heisenberg equation of motion ansatz [4], we discuss the first order of non-linear exciton-phonon interaction exceeding the classical Boltzmann scattering limit, in order to analyze the exciton thermalization at elevated excitation densities.
[1] Wang et al. RMP, 90, 021001 (2018). [2] Selig et al. arXiv:2201.03362 (2022). [3] Chow et al., Nano lett. 17, 1194 (2017); Shree et al. PRB 98, 035302 (2018). [4] Selig et al. PRR, 1, 022007 (2019); Katsch et al., PRL 124 25 257402 (2020).

DS 7.12 Mon 18:15 H36

Ultrafast control of spins in transition metal dichalcogenides — •Abhijeet Kumar[1], Denis Yagodkin[1], Douglas J. Bock[1], Nele Stetzuhn[1,2], Sviatoslav Kovalchuk[1], Alexey Melnikov[3], Peter Elliott[2], Sangeeta Sharma[2], Cornelius Gahl[1], and Kirill I. Bolotin[1] — [1]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born Straße 2a, 12489 Berlin, Germany — [3]Institute for Physics, Martin Luther University Halle, 06120 Halle, Germany

Control and manipulation of the coupled spin/valley degrees of freedom in transition metal dichalcogenides (TMDs) are essential for their applications in spin/valleytronics. Here, we achieve ultrafast control of spins in TMDs via two distinct approaches, namely, proximity-coupling to another TMD and strain. First, we use a type-II heterostructure $MoS_2 - MoSe_2$ to enable directional optical pumping of spin-polarized carriers. We find that the photoexcited carriers conserve their spin for both tunneling directions across the interface. We observe dramatic differences in the spin/valley depolarization rates for electrons and holes, 30 and $<1\ ns^{-1}$, respectively, which relates to the disparity in the spin-orbit splitting in conduction and valence bands of TMDs. Second, by applying biaxial strain (exceeding 2%) in monolayer WSe_2, we evidence the hybridization of the conduction bands with the in-gap localized defects that brightens the lowest-lying dark excitons. This novel hybrid state exhibits unique spin/valley signatures which are strongly manipulated on picosecond-timescale by strain and doping.

DS 8: 2D Materials 3 (joint session CPP/DS)

Time: Monday 17:15–17:45 Location: H38

DS 8.1 Mon 17:15 H38

On the electronic pi-system of 2D covalent organic frameworks — •Konrad Merkel, Johannes Greiner, and Frank Ortmann — TU München

We investigate a family of 2D hexagonal covalent organic frameworks (COFs) with different linker monomers regarding their electronic structure and pi-conjugation. Molecular orbitals can be obtained from maximally localized Wannier functions and turn out to be sigma- and pi-like orbitals forming distinct sigma- and pi-bands, respectively. The Wannier description enables a detailed analysis of the topology, effective coupling and delocalization of the entire pi-system. We identify conjugated states that are delocalized across multiple building blocks of the COF and show their robustness against perturbations like out-of-plane rotations of molecular fragments and different strength of Anderson disorder. Furthermore, we apply the nucleus-independent chemical shift (NICS), which is an established measure of aromaticity. All results are compared for different types of linker units with different degrees of pi-conjugation.

DS 8.2 Mon 17:30 H38

Permeation of gases through molecularly thin carbon nanomembranes — •Vladislav Stroganov[1], Daniel Hüger[1], Tabata Nöthel[1], Christof Neumann[1], Uwe Hübner[2], Michael Steinert[1], Monika Kruk[3], Piotr Cyganik[3], and Andrey Turchanin[1] — [1]Friedrich-Schiller University Jena, Jena, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany — [3]Jagiellonian University, Kraków, Poland

Atomically thin carbon nanomembranes (CNMs) are promising candidates for next generation filtration and gas separation technologies. However, the gas permeation mechanism through CNMs is not fully understood yet. To improve this knowledge, we investigated permeation of helium, deuterium, water vapor and other gases through a series of CNMs under different conditions. The CNMs were synthesized from biphenyl substituted carboxylic acids on silver substrate $C_6H_5 - C_6H_4 - (CH_2)_n - COO|Ag$, with different lengths of aliphatic linker n = 2 - 6. A CNM based on terphenyl thiol (TPT) was used as a well-known reference system. We demonstrated that even the smallest variation in the structure of the molecular precursor lead to significant change of the permeation properties.

DS 9: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 3

Time: Tuesday 9:30–11:00 Location: H14

DS 9.1 Tue 9:30 H14

Structural properties of iron dichalcogenide thin films deposited by selenization process — •Luqman Mustafa[1], Andreas Kreyssig[1], Jill Fortmann[2], Aurelija Mockute[2], Alfred Ludwig[2], and Anna E. Böhmer[1] — [1]Institute for Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, Germany

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

We report on the formation of (Fe,X)Se_2, (X= Co, Mn, Cr....) thin films by ex-situ selenization of amorphous transition metal thin films. Using combinatorial deposition allowed to efficiently explore a wide range of substitution at the iron site with different transition metals (for example Co, Mn, Cr). The dependence of structural properties and phase stability on the selenization temperature and substitution level has been investigated. The process may be adapted for other transition metal dichalcogenides thin films, such as $FeSb_2$, and is therefore a unique tool to study a broad material family and its possible substitution ranges.

DS 9.2 Tue 9:45 H14

Structural and elastic properties of $Sc_xAl_{1-x}N$ — •Saskia Mihalic[1], Armin Dadgar[2], Niclas M. Feil[1], Christopher Lüttich[2], André Strittmatter[2], and Oliver Ambacher[1] — [1]Department of Sustainable Systems Engineering, University of Freiburg, Germany — [2]Department of Semiconductor Epitaxy, Otto von Guericke University Magdeburg, Germany

The hexagonal compound alloy scandium aluminum nitride ($Sc_xAl_{1-x}N$) shows an enhancement of the piezoelectric module $d_{33}(x)$ by more than 300 % compared to aluminum nitride (AlN). Therefore, $Sc_xAl_{1-x}N$ is a highly promising material for the implementation of acoustic resonators for mobile communication systems, although usually a larger stiffness of the material is required. The direction-dependent elastic behavior of hexagonal $Sc_xAl_{1-x}N$ crystals is represented by the reciprocal Young's modulus $S^*_{11}(x)$ and aids in identifying the best trade-off between piezoelectric and elastic properties of anisotropic $Sc_xAl_{1-x}N$ for microacoustic applications. To confirm the calculations with experimental results, thin films of $Sc_xAl_{1-x}N(0001)$ and ScN(111) on Si-substrates were grown by reactive magnetron sputter epitaxy. The structural properties of thin films have been investigated by high-resolution X-Ray diffractometry (HRXRD) and high-resolution transmission electron microscopy (HRTEM). Furthermore, we will present a detailed comparison of

theoretical and experimental results of the piezoelectric and stiffness coefficients achieved by the analysis of $Sc_xAl_{1-x}N$-based SAW resonators.

DS 9.3 Tue 10:00 H14

Structural analysis of $Sc_xAl_{1-x}N$ thin films — •Rebecca Petrich[1], Younes Slimi[1], Hauke Honig[2], Lorenz Steinacker[2], Katja Tonisch[1], Raphael Kuhnen[3], Dietmar Frühauf[3], and Stefan Krischok[1] — [1]TU Ilmenau, FG Technische Physik I, IMN MacroNano, 98693 Ilmenau — [2]TU Ilmenau, FG Werkstoffe der Elektrotechnik, IMN MacroNano, 98693 Ilmenau — [3]Endress+Hauser SE+Co. KG, TTD Technologieentwicklung, 79689 Maulburg

The further and new development of functional materials is an important and constant research approach for the optimization of microelectromechanical systems. In the field of piezoelectric materials, AlN stands out due to its good piezoelectric properties and its CMOS compatibility, its very good thermal stability and high sound velocity. While the basic research for this material is considered to be largely completed, research for the scandium-based alloy $Sc_xAl_{1-x}N$ is still in its infancy. The need for investigation is particularly high for alloys with scandium concentrations of more than x = 15%. For this purpose, $Sc_xAl_{1-x}N$ thin films were deposited and analyzed using pulsed magnetron sputtering in a concentration range between x = 15% and 35%. Starting with the crystal orientation (X-ray diffractometry) and the layer composition (energy-dispersive X-ray spectroscopy) through to the surface roughness (atomic force microscopy), optical parameters for determining the layer thickness and dielectric function (spectroscopic UV-Vis ellipsometry) were also examined and compared to pure AlN. In addition, the homogeneity of the layer properties was examined over different radii on 4" Si wafers.

DS 9.4 Tue 10:15 H14

Phase behavior of dumbbell monolayers obtained via Langmuir-Blodgett-like Brownian dynamics simulations — •Anton Lüders, Rouven Stuckert, Ellen Zander, Alexander Wittemann, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

We explore the structure formation and the phase behavior of thin films of dumbbell colloids. For this, we first determine empiric formulas for the microscopic diffusion coefficients of dumbbells using a bead-shell approach. These diffusion coefficients are used to perform two-dimensional Brownian dynamics (BD) simulations where the area fraction of the system is adjusted via movable barriers at the boundaries of the simulation box. The results of the simulations are compared to Langmuir-Blodgett experiments with dumbbell monolayers at the air/water interface. Using Voronoi diagrams and the Voronoi cell shape factor, the influence of the area fraction on the structure of the monolayers is investigated. The simulations and the experiments show - in excellent agreement with each other - that an increase of the area fraction leads to a higher percentage of domains containing particles with six nearest neighbors. Especially in dense systems, these domains can consist of aligned particles with uniform Voronoi cells. Thus, the increase of the area fraction enhances the order of the monolayers. The remarkable qualitative agreement of the simulations and the experiments indicates a versatile way of characterizing colloidal monolayers by BD simulations which opens up perspectives for application to a broad range of nanoparticle-based thin film coatings.

DS 9.5 Tue 10:30 H14

Thermal Laser Epitaxy of Refractory Metals — •Lena Nadine Majer, Hongguang Wang, Wolfgang Braun, Peter A. van Aken, Jochen Mannhart, and Sander Smink — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

In thermal laser epitaxy, both the substrate and the individual evaporation sources are heated by high-power continuous-wave lasers. This method combines the advantages of MBE and PLD, allowing the efficient thermal evaporation and epitaxial deposition of practically any combination of elements from the periodic table. We demonstrate and discuss the epitaxial growth of refractory metals on c-cut sapphire. As examples we present Ru and Ta growth, because they are of particular interest for many technological applications. We have optimized the growth parameters to obtain epitaxial films of superior quality, which are apparently devoid of defects over large areas. The films have been characterized by AFM, RHEED, STEM, and X-ray analysis, revealing that the layers grow single phase, with a low surface roughness and that the interface between the layer and the substrate is atomically sharp.

DS 9.6 Tue 10:45 H14

Temperature-dependent C-AFM measurements on rhodium paddle-wheel coordination polymers — Daniel Steinbach, Sophie Gersdorf, and •Florian Mertens — Institute of Physical Chemistry, TU Bergakademie Freiberg, Germany

To overcome one of the disadvantages of most coordination polymers and metal-organic frameworks being insulators, conjugated coordination polymers are investigated regarding their electrical conductivity. To obtain a potentially conductive system paddle-wheel structures with a documented metal-metal bond, here rhodium derivates, were linked via conjugated organic molecules like pyrazine. Coordination polymers of this type were first synthesized as bulk materials, characterized using XRD, TG-DSC and XPS and then deposited as coatings on gold surfaces. Subsequently, the topography of the deposited layers was determined. The morphological properties of the coatings were correlated with the properties of the basic coordination polymer components.

The conductivity was investigated via temperature-dependent C-AFM measurements. As expected no conductivity is measurable for coordination polymers containing acetates based paddle-wheels even if they are linked with a tridentate conjugated ligand. For the $[Rh_2(acam)_4(pyz)]_n$ (Hacam = acetamide) coordination polymer a strong temperature and field dependency of the conductivity was observed. From the corresponding measurements an arrhenius type activation energy of app. 0.3-0.4 eV was derived. In addition, various conduction mechanisms were discussed.

DS 10: Gaede Prize Talks

Time: Tuesday 9:30–11:30 Location: H17

Laudatio

Prize Talk DS 10.1 Tue 9:40 H17

Atomic-Scale Optical Spectroscopy at Surfaces — •Takashi Kumagai — Fritz Haber Institute, Berlin, German — Institute for Molecular Science, Okazaki, Aichi, Japan — Laureate of the Gaede-Prize 2020

Light-matter interactions can be largely enhanced in the presence of optical near fields. Atomic-scale light-matter interactions in plasmonic "picocavities" has emerged as a new frontier of fundamental light science and technology [1]. However, the investigation of such light-matter interactions still involves significant challenges in both experiment and theory. A combination of plasmon-enhanced spectroscopy with low-temperature STM can provide a unique way to investigate intriguing physics resulting from the strong interaction between cavity-mode plasmon and matter even at atomic scales [2]. I will discuss our recent development toward atomic-scale optical spectroscopy in plasmonic STM junctions [3].

References: [1] Nat. Mater. 18, 668 (2019). [2] Nat. Rev. Phys. 3, 411 (2021). [3] Phys. Rev. Lett. 128, 206803 (2022); Nano Lett. 22, 2170 (2022); ACS Photonics 8, 2610 (2021); Nano Lett. 21, 4057 (2021); Nano Lett. 20, 5879 (2020); Nano Lett. 19, 5725 (2019); Nano Lett. 19, 3597 (2019).

Laudatio

Prize Talk DS 10.2 Tue 10:20 H17

Slow highly charged ions as a tool for monolayer sensitive nano-engineering — •Richard Wilhelm — TU Wien, Institute of Applied Physics, Vienna, Austria — Laureate of the Gaede-Prize 2021

Heavy ions in high charge states can be prepared with kinetic energies in the keV energy range. These slow ions interact with surface electrons upon impact of a material which leads to their neutralisation and

consequently to the deposition of several ten keV of potential energy. Over the past 20 years it has been a puzzle how fast and consequently how surface sensitive this energy deposition is. With the use of free-standing two-dimensional materials we can now limit the interaction time of the ions with a solid to the femtosecond regime. We find that most of the neutralisation of the ions takes place in a single atomic monolayer of material. In this contribution I will discuss recent advancements in the study of ion neutralisation dynamics inside of solids as well as the efficiency of potential energy driven sputtering of atoms. The latter depends on the type of material and can be confined to a single monolayer only, despite the high amount of deposited energy.

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Prize Talk DS 10.3 Tue 11:00 H17

Quantum Science with Single Atoms and Molecules on Surfaces — •Philip Willke — Karlsruhe Institute of Technology, Physikalisches Institut, Karlsruhe, Germany — Laureate of the Gaede-Prize 2022

The quantum nature of a physical system often emerges from its fundamental building blocks and demands a profound understanding to harvest its advantages for quantum devices. In this talk, I will introduce a new architecture for coherent control of spins on surfaces, by combining electron spin resonance (ESR) and scanning tunneling microscopy (STM) [1]. This technique allows to address single atoms and molecules on surfaces with unprecedented energy resolution. Thus, it can be used to sense the magnetic coupling between spin centers on the nanoscale [2]. In addition, when scanning the STM tip across the surface it permits to perform magnetic resonance imaging on the atomic scale [3]. The high energy resolution also grants access to the hyperfine interaction between the electron and nuclear spin of different atomic species [4]. Recently, we could extend this technique also to spin resonance on individual molecules [5]. Lastly, by employing pulsed ESR schemes, a coherent manipulation of the surface spin becomes possible, for instance in Rabi and Hahn echo schemes [6]. This opens up a path towards quantum information processing and quantum sensing using atomic building blocks, including atoms and molecules. [1] S. Baumann et al., Science 350 (2015) [2] T. Choi et al. Nat. Nano 12 (2017) [3] P. Willke et al., Nat. Phys. 15 (2019) [4] P. Willke et al., Science 362 (2018) [5] X. Zhang et al., Nat. Chem. 14 (2022) [6] K. Yang et al., Science 366 (2019)

DS 11: Focus Session: Quantum Properties at Functional Oxide Interfaces 1 (joint session HL/DS)

Modern oxide materials exhibit a rich variety of physical properties that lead to potential applications such as sensors and detectors, solar energy harvesting, transparent and power electronics. Understanding their quantum properties at surfaces and interfaces may play a decisive role for functionalities in high-electron-mobility transistors, quantum electronics or topological quantum computation. These typically require homo- or heteroepitaxial layers of high crystallinity and investigation methods designed to reveal the fascinating physics at (complex) oxide interfaces. This session sets a focus on growth of oxide interfaces, the experimental and theoretical investigation of their novel physical, in particular quantum properties as well as fabrication and characterization of demonstrator devices.

Organized by Martin Albrecht, Oliver Bierwagen, and Saskia F. Fischer

Time: Tuesday 9:30–12:45 Location: H34

Invited Talk DS 11.1 Tue 9:30 H34

Materials and Device Engineering for Gallium Oxide-based Electronics — Nidhin Kurian Kalarickal[1], Sushovan Dhara[1], Ashok Dheenan[1], and •Siddharth Rajan[1,2] — [1]ECE Department, The Ohio State University — [2]MSE Department, The Ohio State University

This presentation will discuss our recent work on epitaxy, heterostructure design, and electrostatics to achieve high-performance β-Ga2O3 lateral and vertical electronic devices. We will discuss some key results in materials growth and device design for lateral structures, including the first β-(Al,Ga)2O3/β-Ga2O3 modulation-doped structures with excellent transport properties, double-heterostructure modulation-doped structures, and scaled delta-doped transistors with cutoff frequency of 27 GHz, and self-aligned lateral field effect transistors with $>$ 900 mA/mm current density. We will discuss the use of a new damage-free epitaxial etching technique using Ga atomic flux that enables highly precise fabrication of 3-dimensional structures, and applications of this etching to realize field termination in vertical diodes, and lateral FINFETs with enhanced performance. Extreme-permittivity dielectrics provide unique opportunities to create devices that can sustain extreme fields without premature breakdown of metal-semiconductor and dielectric-semiconductor interfaces. We will discuss promising results of electrostatic engineering using BaTiO3/Ga2O3 heterojunctions that enable high fields to be sustained within Gallium Oxide diodes and transistors.

Invited Talk DS 11.2 Tue 10:00 H34

Ferroelectric two-dimensional electron gases for oxide spin-orbitronics — •Julien Bréhin — Unité Mixte de Physique CNRS/Thales

Just as the apparent incompatibility between ferroelectricity and magnetism prompted the renaissance of multiferroics, the research on ferroelectric metals conjectured in the 1960s by Anderson and Blount was recently revitalized. Yet, their experimental demonstration remains very challenging due to the contra-indication between the presence of free charge carriers and switchable electric dipoles. In this talk we will report on two-dimensional electron gases (2DEGs) formed on Ca-substituted SrTiO3 (STO). Signatures of the ferroelectric phase transition near 30 K are visible in the temperature dependence of the sheet resistance RS and in a strong, reproducible hysteresis of RS with gate voltage. In addition, spectroscopic measurements of the 2DEG region indicate the presence of switchable ionic displacements. Beyond their fundamental interest in materials physics, ferroelectric 2DEGs offer opportunities in spin-orbitronics: we will show how their spin-charge conversion properties, caused by the inverse Rashba-Edelstein effect, can be electrically tuned in amplitude and sign in a non-volatile way. These results open the way to a whole new class of ultralow-power spin-orbitronic devices operating without the need for magnetization switching. Finally, we will describe how one can introduce magnetism into such systems to achieve multiferroic 2DEGs displaying magneto-electric coupling.

DS 11.3 Tue 10:30 H34

Electron transport of the two-dimensional electron gas in polar-discontinuity doped LaInO3/BaSnO3 heterostructure — Georg Hoffmann[1], Fazeel Zohair[1], Martina Zupancic[2], Martin Albrecht[2], and •Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung im Forschungsverbund Berlin e.V., Max-Born-Straße 2 D-12489 Berlin, Germany

Transparent semiconducting oxides (TSOs) are key players for new (opto-)electronic devices and two-dimensional electron gases (2DEGs) are relevant for high-frequency applications. Polar-discontinuity doping (interfacing a polar material with a nonpolar one), has been demonstrated to provide a 2DEG at the interface between the perovskites LaAlO3 and SrTiO3 with a high electron concentration but suffers from low room-temperature (RT) electron mobilities of SrTiO3. In this contribution we demonstrate polar-discontinuity doped 2DEG at the interface between the perovskites LaInO3 and BaSnO3, grown

by plasma-assisted molecular beam epitaxy. While the individual, undoped oxide layers were found to be insulating, the formation of the polar-discontinuity doped 2DEG at their interface is confirmed by capacitance-voltage (CV) and van der Pauw-Hall measurements. The extracted sheet electron concentrations >2e13cm^-2 and RT electron mobilities above >50cm^2/Vs are promising for device applications. The transport properties of the 2DEG are compared to those of La-doped BaSnO3 layers.

DS 11.4 Tue 10:45 H34

Non-Abelian braiding of phonons in monolayer oxides — •Bo Peng[1], Adrien Bouhon[1], Bartomeu Monserrat[1,2], and Robert-Jan Slager[1] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

Non-Abelian braiding of quasiparticles can encode quantum information immune from environmental noise with the potential to realize topological quantum computation. Here we propose that phonons, a bosonic excitation of lattice vibrations, can carry non-Abelian charges in their band structures that can be braided using external stimuli. Taking some earthly abundant materials such as silicates [1] and aluminium oxide [2] as representative examples, we demonstrate that an external electric field or electrostatic doping can give rise to phonon band inversions that induce the redistribution of non-Abelian charges, leading to non-Abelian braiding of phonons. We show that phonons can be a primary platform to study non-Abelian braiding in the reciprocal space, and we expand the toolset to study such braiding processes.

References: [1] Bo Peng, Adrien Bouhon, Bartomeu Monserrat & Robert-Jan Slager. Nature Communications 13, 423 (2022). [2] Bo Peng, Adrien Bouhon, Robert-Jan Slager & Bartomeu Monserrat. Physical Review B 105, 085115 (2022).

30 min. break

DS 11.5 Tue 11:30 H34

Shift of the absoption onset in corundum-like α-$(Ti_xGa_{1-x})_2O_3$ — •Elias Kluth[1], Michael Fay[2], Christopher Parmenter[3], Joseph Roberts[4], Fabien Massabuau[5], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, NG7 2RD, UK — [3]Nottingham Nanotechnology and Nanoscience Centre, University of Nottingham, University Park, Nottingham NG7 2RD, UK — [4]School of Engineering, The University of Liverpool, Liverpool L69 3GH, UK — [5]Department of Physics, SUPA, University of Strathclyde, Glasgow G4 0NG, UK

Corundum-like α-Ga_2O_3 is a metastable phase of the polymorphic ultra-wide band gap semiconductor Ga_2O_3. While previous resarch has mostly focused on the stable β-phase the α-phase is less discussed, but interesing as well as it allows bandgap-engineering by alloying e.g. with α-Al_2O_3 (sapphire) or In_2O_3.
Since the transition metal oxide Ti_2O_3 as well, has a corundum-like phase (α-phase), with a small latice mismatch of about 3.5% to α-Ga_2O_3, we investigate here (0001) α-Ga_2O_3 thin films alloyed with Ti, grown by ALD (atomic layer deposition).
We use spectroscopic ellipsometry in ultraviolet range to obtain the complex dielectric function (DF) of α-$(Ti_xGa_{1-x})_2O_3$ up to $x = 0.61$. We find a clear red shift of the absorption onset with increasing Ti content, as well as an increase of the amplitude of the DF.

DS 11.6 Tue 11:45 H34

Optical signatures of polarons trapped at ferroelectric domain walls in bismuth ferrite — •Sabine Körbel — Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — Friedrich Schiller University Jena, Germany

Ferroelectric domain walls are atomically narrow planes that can behave very differently from the surrounding bulk ferroelectric material. For example, the domain walls in many ferroelectrics can collect and conduct charge carriers despite the insulating nature of the host material. Domain walls can be created, moved, and removed again in a controlled way, thus they can be used to alter the electronic properties of the ferroelectric as desired. Charge carriers that accumulate at domain walls may induce metallic or semiconducting behavior depending on whether they are delocalized or form self-trapped small polarons. The latter may be detected, for example, as deep levels within the band gap in absorption or photoluminescence spectra. Here we predict optical signatures of charge carriers trapped as small polarons at ferroelectric domain walls in $BiFeO_3$, using first principles calculations.

DS 11.7 Tue 12:00 H34

Anharmonicity of lattice vibrations in α-Ga_2O_3 investigated by temperature dependent Raman spectroscopy — •Jona Grümbel[1], Rüdiger Goldhahn[1], Dae-Woo Jeon[2], and Martin Feneberg[1] — [1]Otto-von-Guericke Universität, Magdeburg, Germany — [2]Korea Institute of Ceramic Engineering and Technology, Jinju, Republic of Korea

We investigate the Raman excitations of a corundum-like α-Ga_2O_3 thin film under temperature variation from 80K up to 790K. This yields detailed information about anharmonic processes in the crystal. For the two dominant phonon modes for each of the two Raman-active phonon mode symmetries (A_{1g} and E_g) model calculations are performed in order to quantify the contributions of different decay mechanisms. It is shown, that our experimental data can be well described by the applied theoretical models. The determined coefficients of cubic and quartic decay for both, phonon energy and linewidth, are compared with those from hexagonal GaN and AlN as well as with those from α-Al_2O_3. We observe, that for the two selected phonon modes of α-Ga_2O_3 the quartic decay processes are negligible for the phonon frequencies, but not for the phonon linewidths behavior under temperature variation. A quantitative description within the model parameters is presented.

Invited Talk DS 11.8 Tue 12:15 H34

Strain-driven dissociation of water on (incipient) ferroelectrics — Joshua L. Bates and •Chiara Gattinoni — Department of Chemical and Energy Engineering, London South Bank University, London, UK

Functional materials have great promise in catalysis, and especially within dynamic catalytic cycles, where the "functional" properties are used to cyclically modify the local environment of a surface to enhance turnover frequency. In particular, strain-driven mechanisms exploiting the properties of piezo- and ferroelectric materials, are of great interest.

In this work we focus on (incipient) ferroelectric nanomaterials $BiFeO_3$, $BaTiO_3$, $KTaO_3$ and $SrTiO_3$, perovskites presenting a wide range of bulk properties and behaviours. We uncover how interplay between these properties (such as the spontaneous polarization) and nanoscale effects (such as the depolarizing field and the surface structure), affect the strain-driven water-splitting abilities of these nanoscale functional materials. Finally, we identify the most desirable properties for a highly efficient ferroelectric material for dynamic catalysis.

DS 12: 2D Materials 4 (joint session HL/CPP/DS)

Time: Tuesday 9:30–12:00 Location: H36

Invited Talk DS 12.1 Tue 9:30 H36

Ultrafast all-optical modulation and frequency conversion in 2D materials — •Sebastian Klimmer[1], Artem Sinelnik[1,2], Isabelle Staude[1,2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Germany

Large efforts have been devoted in the last years to realizing nonlinear integrated devices for frequency conversion, sensing, signal modulation and quantum optics. Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), provide distinct advantages in this respect thanks to their ease of integration on photonic platforms[1] and their atomically thin nature, which relaxes phase matching constraints and thus offers a practically unlimited bandwidth for nonlinear optical effects [2]. In this seminar I will present our recent results in the field of nonlinear optics with 2D materials, including ultra-broadband four-wave mixing in the telecom range, ultrafast all-optical modulation of second- and third-harmonic generation in TMDs[3] and graphene and ultrafast polarization-resolved second-harmonic spectroscopy to probe the valley degree of freedom in TMDs.

[1] He, J. *et al.*, Nano Lett. **21**, 7, 2709-2718 (2021)
[2] Trovatello, C. *et al.*, Nat. Photonics. **15**, 6-10 (2021)
[3] Klimmer, S. *et al.*, Nat. Photonics. **15**, 837-842 (2021)

DS 12.2 Tue 10:00 H36

strain tuning of exciton and trion dynamics in monolayer WSe2 at cryogenic temperatures — •zhao an[1], pedro soubelet[2], andreas v. stier[2], michael zopf[1], yaroslav zhumagullov[3], jaroslav fabian[3], paulo e. faria jonior[3], jonathan j. finley[2], and fei ding[1,4] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, 85748 Garching, Germany — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [4]Laboratorium fur Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Transition metal dichalcogenides (TMD) receive increasing attention these years. In TMD monolayers, the light-matter interaction is driven by strong excitonic effects. Additional to neutral excitons, singlet/ triplet trions are observed, in which the additional charge is either in the same or opposite valley with respect to excitons. We apply dynamic strain at cryogenic temperatures to investigate the exciton dynamics of monolayer WSe2. Biaxial strain is electrically controlled via a piezoelectric actuator and transferred to the hBN/WSe2/hBN. We find that next to changes in the emission energy and intensity, the singlet-triplet trion fine structure is affected. Polarization-resolved PL spectroscopy reveals that biaxial strain alters the polarizations of trions, which is attributed to changes in the pumping of resident electrons and the intervalley scattering of excitons and electrons.

DS 12.3 Tue 10:15 H36

Optical nonlinearities in the excited carrier density of 2d TMDs — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Bremen Center for Computational Materials Science, University of Bremen

The prospects of using 2d transition metal dichalcogenides (TMDs) in future optoelectronic device application requires insight in the excitation dynamics of photoexcited charge carriers and the resulting optical nonlinearities. Utilizing ab-initio electronic-state calculations combined with many-body treatment of optical excitation, we calculate the excited carrier dynamics and the nonlinear absorption in MoS_2, $MoSe_2$, WS_2, and WSe_2 under various excitation conditions.
We find, that the increase of the carrier density with excitation strength deviates from a linear behaviour. Based on this, the validity range of a linear approximation for the excited carrier density as function of the pump fluence is determined. The use of a linear absorption coefficient of the unexcited system can significantly underestimate the achievable carrier density for strong pump fields. Furthermore, we study the excitation-induced many-body effects of excited charge carriers like band-gap renormalization, dephasing, screening, and scattering processes, that are mediated by the strong Coulomb interaction. Additional contributions to optical nonlinearities originate from phase space filling.

15 min. break

DS 12.4 Tue 10:45 H36

Second order coherence of a condensate of exciton-polaritons in an atomically thin crystal — •Jens-Christian Drawer[1], Hangyong Shan[1], Sven Höfling[2], Carlos Anton-Solanas[3], Martin Esmann[1], and Christian Schneider[1] — [1]Universität Oldenburg, Germany — [2]Universität Würzburg, Germany — [3]Universidad Autónoma de Madrid, Spain

We study the second order coherence of a condensate of exciton-polaritons emerging in a microcavity loaded with an atomically thin $MoSe_2$ crystal. Under cryogenic temperatures, angle-resolved PL and reflectivity measurements reveal the formation of two polariton resonances, as the hallmark of the strong coupling regime. The characteristic condensation threshold manifests via the nonlinear input-output-characteristics of the emission. In order to gain deeper information about the photon statistics emitted from the cavity, we perform the Hanbury Brown- and Twiss experiment as a function of the polariton occupation in the effective ground state. While the emission features a bunching effect below threshold, hinting at a thermal contribution of the polariton emission, above threshold the second order correlation transits towards $g^{(2)}(\tau = 0) = 1$, which is indicative for the formation of a coherent state in the quantum optical sense.

DS 12.5 Tue 11:00 H36

Theoretical description of moiré excitons in twisted $MoSe_2$ homobilayers — •Ruven Hübner[1], Malte Kremser[2], Viviana Villafañe[2], Marko M. Petrić[3], Matthias Florian[4], Alexander Steinhoff[1], Mackillo Kira[4], Nathan P. Wilson[2], Andreas V. Stier[2], Kai Muller[3], and Jonathan J. Finley[2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [3]Walter Schottky Institut and Department of Electrical and Computer Engineering, Technische Universität München, Garching, Germany — [4]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

By introducing a twist between multiple monolayers of transition metal dichalcogenides we can observe superstructures with a new periodicity - namely the moiré lattice. Its size depends on the twist angle and therefore offers the possibility to modify properties like exciton energies as a function of the twist angle. We demonstrate, how DFT calculations of an untwisted $MoSe_2$ bilayer allow us to locally model the band variation inside the moiré unit cell at all dominant high symmetry points of the Brillouin zone. The resulting model provides access to arbitrary moiré potentials experienced by different exciton species and allows us to calculate their twist angle dependent spectra. For all twist angles we assign the lowest energy to interlayer excitons formed between the Γ- and K-valley. The twist angle dependent shift of 5 meV per degree for small angles is in good agreement with experiment.

DS 12.6 Tue 11:15 H36

Dielectric screening effects on the exciton binding-energy and exciton diffusion in a 2D material — •Lukas Gümbel, Philip Klement, and Sangam Chatterjee — Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, Giessen D-35392, Germany

Two-dimensional semiconductors have proven to be candidates for numerous applications in the field of optoelectronics. Especially transition-metal dichalcogenides such as WS_2 have attracted extensive research due to the direct band-gap emerging in the monolayer limit. The optoelectronic properties are dominated by tightly-bound excitons denoted as A, B, and C. As the electric field lines of the excitonic states extend into the surrounding material, the energy states are subject to dielectric screening effects. Here we show that stronger dielectric screening equally shifts the excitonic ground state energies

of the A-, B-, and C-excitons in WS_2 to lower energies. We find a shift of 20 meV in monolayers encapsulated in hBN and observe a non-hydrogenic Rydberg-series yielding a quasiparticle band-gap energy of 2.33 eV with an 1s excitonic binding energy of 0.30 eV. Additionally, we study exciton diffusion in different dielectric environments yielding a diffusion coefficient of 9 cm^2/s. These results complement the underlying theory and may pave the way to a deeper understanding of screening effects in various 2D-Materials.

DS 12.7 Tue 11:30 H36

Brightening of a dark monolayer semiconductor via strong light-matter coupling in a cavity — •Hangyong Shan[1], Ivan Iorsh[2], Bo Han[1], Falk Eilenberger[4], Martin Esmann[1], Sebastian Klembt[3], Sven Höfling[3], Carlos Antón-Solanas[1], Ivan A. Shelykh[2], and Christian Schneider[1] — [1]Oldenburg University, Oldenburg, Germany. — [2]St. Petersburg, Russia — [3]Universität Würzburg, Würzburg, Germany — [4]Friedrich Schiller University, Jena, Germany

We study the modification of the material properties via strong coupling and demonstrate an effective inversion of the excitonic band-ordering in a monolayer of WSe2 with spin-forbidden, optically dark ground state. In our experiments, we harness the strong light-matter coupling between cavity photon and the high energy, spin-allowed bright exciton, and thus creating two bright polaritonic modes in the optical bandgap with the lower polariton mode pushed below the WSe2 dark state. We demonstrate that in this regime the commonly observed luminescence quenching stemming from the fast relaxation to the dark ground state is prevented, which results in the brightening of this intrinsically dark material. We probe this effective brightening by temperature-dependent photoluminescence, and we find an excellent agreement with a theoretical model accounting for the inversion of the band ordering and phonon-assisted polariton relaxation.

DS 12.8 Tue 11:45 H36

Broadband pump-probe microscopy at 1.5 MHz repetition rate — •Devapriyo Mithun[1], Michael Frosz[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany

Ultrafast pump-probe spectroscopy is one of the most commonly used techniques to resolve photoinduced excited states dynamics: a pump pulse excites the system under investigation, which is then monitored by measuring the changes in the differential reflection ($\Delta R/R$) of a temporally delayed probe pulse. Here, we discuss the realization of a pump-probe setup, which exhibits high sensitivity operating with a temporal resolution of $\approx$ 100 fs and spatial resolution of $\approx$ 3 μm with 515 nm pump and a broadband probe spectrum in the range 650-1000 nm, generated with a photonic crystal fiber.

We modulate the pump pulse at 1.5 MHz using an acousto-optic modulator. By doing this, we achieve a sensitivity, defined as the minimum detectable $\Delta R/R$, of 10^{-7} at 10 ms integration time. Finally, we implemented a Fourier transform based interferometric detection scheme to achieve a fast measurement of $\Delta R/R$ over the entire broadband spectrum.

Our pump-probe setup provides a powerful tool for broadband pump-probe microscopy with high sensitivity and high temporal resolution, which is ideal for the study of nanostructures such as carbon nanotubes and layered materials.

DS 13: Thin Film Applications 2

Time: Wednesday 9:30–10:45 Location: H14

DS 13.1 Wed 9:30 H14

Investigation of Production Techniques for Sputtered Tungsten Thin Films — •Tobias Ortmann[1], Andreas Erhart[1], Margarita Kaznacheeva[1], Angelina Kinast[1], Alexander Langenkämper[1], Luca Pattavina[1], Walter Potzel[1], Johann Riesch[2], Johannes Rothe[1], Nicole Schermer[1], Stefan Schönert[1], Raimund Strauss[1], Victoria Wagner[1], and Alexander Wex[1] — [1]Technische Universität München, Physik Department Lehrstuhl E15, James-Franck-Straße 1, D-85748 Garching — [2]Max-Planck-Institut für Plasmaphysik, Boltzmannstraße 2, D-85748 Garching bei München

Cryogenic rare event searches like the CRESST and the NUCLEUS experiments use TES (Transition Edge Sensors) as phonon sensors to read out their target crystals. This type of sensors utilizes the superconducting phase transition of tungsten to measure the energy deposited in the absorbers. The most established method of production for these films is electron beam physical vapor deposition. For future large scale production the application of argon DC-magnetron sputtering is investigated in terms of film quality and reproducibility. The most recent results of these investigations are presented. The research was supported by the DFG through the Excellence Cluster ORIGINS and the SFB1258, and the BMBF: 05A17WO4 and 05A17VTA.

DS 13.2 Wed 9:45 H14

Preparation of $RuVO_2$ alloy thin films and theirs uncooled infrared detection performance — •Hao Lu[1,2,3], Yunbin He[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]School of Materials Science and Engineering, Hubei University, Wuhan 430062, China

Vanadium dioxide (VO_2) films are the most popular materials for sensing layers in uncooled IR detectors because of their high TCR of -2.0 %/K, low noise, low thermal conductivity. The monoclinic phase (M1) of VO_2 undergoes an insulator-to-metal transition at 341K which is accompanied by the crystal structure changing from tetragonal to rutile. The structural phase transition exhibits a thermal hysteresis, which reduces the sensitivity of the minimum temperature change detectable indicative for the IR intensify. So we focused on decreasing the thermal hysteresis width whilst increasing TCR, and carried out the following study: (022) oriented $RuVO_2$ alloy thin films were prepared on TiO_2 (110) substrates by pulsed laser deposition. It was found that the thermal hysteresis width of $RuVO_2$(M1) for Ru content contents above 7% is smaller than for corresponding binary VO_2. The TCR of such $RuVO_2$ alloy films was -5.2%/K, and the thermal hysteresis was no longer observable from electrical properties. This work demonstrates the potential of VO_2 (M1) for the development of the IR detector.

DS 13.3 Wed 10:00 H14

Tracking the evolution of polarization in $BiFeO_3$-based devices — •Marvin Müller[1], Yen-Lin Huang[2], Saül Vélez[3], Ramamoorthy Ramesh[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Department of Material Science and Engineering, University of California, Berkeley, USA — [3]Department of Physics, Universidad Autónoma de Madrid, Spain

The integration of magnetoelectric multiferroics, hosting coexisting and coupled ferromagnetic and ferroelectric orders, into magnetoelectric spin-orbit logic devices holds promises for unprecedented performance and reduction of energy consumption by several orders of magnitude. While static properties such as the coercive electric field have been thoroughly studied and optimized, investigations on the evolution of the ferroic orders during electric-field switching cycles are sparse.

Here, we study the three-dimensional evolution of the net polarization in the technologically highly relevant magnetoelectric material $La_{0.15}Bi_{0.85}FeO_3$. Using optical second-harmonic generation microscopy, we access the polarization of the films integrated in capacitor heterostructures operando. We demonstrate that electric-field training results in a spontaneous domain ordering and a giant enhancement of the net in-plane polarization in $La_{0.15}Bi_{0.85}FeO_3$. Finally, we distinguish between the behavior of the in-plane and out-of-plane polarization during the electric poling. Our investigations thus give unprecedented insights into the polarization dynamics in integrated $BiFeO_3$-based devices.

DS 13.4 Wed 10:15 H14

Photoelectrochemical properties of CuBi2O4-based electrodes prepared via spin-coating for solar water splitting. — •Francesco Caddeo, Marco Krueger, Sophie Medicus, Carina Hedrich, Robert Zierold, and Dorota Koziej — University of Hamburg, Institute of Nanostructure and Solid State Physics Luruper

Chaussee 149, D-22761 Hamburg, Germany

Photoelectrochemical (PEC) water splitting is one of the most promising technologies for the conversion of solar energy into hydrogen gas, which can be stored and used on demand as a fuel with net-zero CO2 emissions. Copper bismuth oxide (CuBi2O4) is recently emerging as a promising metal-oxide to be used as a light harvesting material in the photocathode of a PEC cell and is attracting increasing attention due to its well-suited bandgap of ca. 1.8 eV, its conduction band position of -0.7 V vs RHE (Reversible Hydrogen Electrode) and its highly anodic onset potential of ca. 0.8 V vs RHE, which makes it an ideal material to be implemented in a tandem device for unassisted solar water splitting. In our labs, we have developed a spin-coating procedure that allows us to fabricate highly uniform CuBi2O4 films with pure crystalline phase and various thicknesses on top of fluorine-doped tin oxide coated glass (FTO) used as a support. During my presentation, I will talk about recent results on the synthesis, characterization and photoelectrochemical properties of CuBi2O4 based photo-electrodes protected with a uniform coating of TiO2 overlayer deposited using Atomic Layer Deposition (ALD).

DS 13.5 Wed 10:30 H14

Growth and electrical properties of sputtered gallium oxide device — •Aman Baunthiyal, Marco Schowalter, Thorsten Mehrtens, Andreas Rosenauer, Seyed Majid Mahdian, Jon-Olaf Krisponeit, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Due to the scalability limitations of conventional semiconductor based devices, there is a high demand for powerful memory devices. Resistive switching (RS) is a promising phenomenon especially for future resistance random access memories. In the last few years, gallium oxide has attracted the interest of researchers toward RS applications due to its very large breakdown voltage and concentration sensitive to oxygen content. In this work, we present devices with RF sputtered gallium oxide on ultra smooth Ru/Al_2O_3 for non-volatile RAMs.

Sputter deposition of gallium oxide on $Ru(0001)/Al_2O_3$ at 400°C results in the good crystallinity with diffraction spots matching the β-Ga_2O_3 structure as confirmed by transmission electron diffraction (TED). For device completion, top electrodes (TE) were fabricated by depositing Al/Ag using the e-beam evaporation. X-ray photoelectron spectroscopy (XPS) confirmed a very large amount of oxygen vacancies in gallium oxide film. A RS behaviour in Al TE devices with an ON/OFF ratio of more than 10^4 is suggested to be related to formation/rupture of oxygen vacancies filaments. In the case of Ag TE devices, RS is assigned to electro-metallization of Ag electrode. The stable endurance cycle and long retention time of $> 10^4$ seconds qualify these devices as a future prototype for non volatile ReRAMs.

DS 14: Focus session: Quantum Properties at Functional Oxide Interfaces 2 (joint session DS/HL)

Time: Wednesday 9:30–11:00 Location: H17

Invited Talk DS 14.1 Wed 9:30 H17

Facet dependence of reconstructions at quantum material interfaces — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Oxide heterostructures promise a rational design of quantum materials with specific, functional properties such as magnetism and superconductivity. Our research aims to gain a fundamental understanding of spin, orbital, charge and lattice reconstructions at complex transition-metal oxide interfaces, mainly using x-ray spectroscopy.

In my talk, I will focus on implications of the choice of the crystallographic facet of the interface by showing examples of two prototypical correlated-electrons materials. In $NdNiO_3$ epitaxial thin films we observe modifications of the metal-insulator transition, which we explain by the facet dependence of the bond-order instability in the system [1]. The choice of a specific interface facet, in turn, allows to manipulate the complex spin order in ultrathin $NdNiO_3$ slabs [2]. In YVO_3 heterostructures, an artificial, layered orbital occupation pattern can be realized by the choice of the interface facet [3]. I have conducted the above-mentioned studies in collaboration with many scientists who are co-authors of the publications listed below.

[1] Y. E. Suyolcu, K. Fürsich *et al.*, Phys. Rev. Materials **5**, 045001 (2021). [2] M. Hepting *et al.*, Nature Physics **14**, 1097 (2018). [3] P. Radhakrishnan *et al.*, Phys. Rev. B **104**, L121102 (2021); Phys. Rev. B **105**, 165117 (2022).

DS 14.2 Wed 10:00 H17

A detailed interface and surface analysis of $BaSnO_3$ in $LaInO_3/BaSnO_3$ heterostructures — •Martina Zupancic[1], Wahib Aggoune[2], Daniel Pfützenreuter[1], Zbigniew Galazka[1], Houari Amari[1], Claudia Draxl[2], Jutta Schwarzkopf[1], and Martin Albrecht[1] — [1]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [2]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

$LaInO_3/BaSnO_3$ heterostructures have lately attracted a lot of interest due to the high electron mobility of $\sim 300 cm^2/Vs$ in $BaSnO_3$ and the formation of a 2DEG at the interface. In $LaAlO_3/SrTiO_3$ system, the origin of the 2DEG is attributed to the polar discontinuity and an electronic reconstruction at the n-type LaO-TiO_2 interface. Controlling the interface termination is therefore crucial to accomplish heterostructures with desired properties. Here, we combine density-functional theory, atomic resolution transmission electron microscopy, energy dispersive X-ray spectroscopy, and electron energy loss spectroscopy (EELS) to study the $LaInO_3/BaSnO_3$ interface. Experiment and theory are in excellent agreement and show that free $BaSnO_3$ (100) surfaces are BaO terminated, while the interface between $BaSnO_3$ and $LaInO_3$ is SnO_2 terminated. This finding indicates that during the growth of $LaInO_3$ layer on $BaSnO_3$ Ba atoms exchange from the subsurface to the surface. Preliminary EELS analysis of a few monolayer thick $LaInO_3$ grown on $BaSnO_3$ shows indications of Ba atoms on the $LaInO_3$ surface, confirming that atomic exchange in this system promotes the energetically favorable SnO_2-LaO interface.

Invited Talk DS 14.3 Wed 10:15 H17

Designing novel electronic phases at oxide interfaces from first principles — •Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany

Transition metal oxide interfaces exhibit a rich plethora of functional properties that are not available in the respective bulk compounds and open possibilities for electronics, spintronics and energy conversion applications. Over the past years several control parameters of novel behavior have been identified and systematically explored such as the symmetry breaking at the interface, the effect of strain, confinement and crystallographic orientation, the electrostatic doping at polar interfaces [1]. Based on the insight from density functional theory calculations including an on-site Hubbard term, I will address the formation of unanticipated charge, spin and orbital reconstructions in perovskite-derived superlattices and thin films with (001) and (111) orientation that can lead to e.g. metal-to-insulator transitions and/or topologically nontrivial states which are fascinating not only from a fundamental point of view but also potentially interesting for thermoelectric applications [2].

Research supported by the German Research Foundation DFG within CRC/TRR80. [1] M. Lorenz et al., J. Phys. D: Appl. Phys. 49, 433001 (2016). [2] B. Geisler, P. Yordanov, M. E. Gruner, B. Keimer, R. Pentcheva, Phys. Status Solidi B 259, 2100270 (2022)

DS 14.4 Wed 10:45 H17

Orbital engineering in vanadate heterostructures — •Padma Radhakrishnan[1], Benjamin Geisler[2], Katrin Fürsich[1], Daniel Putzky[1], Yi Wang[1], Sven Ilse[3], Georg Christiani[1], Gennady Logvenov[1], Peter Wochner[1], Peter van Aken[1], Eberhard Goering[3], Rossitza Pentcheva[2], and Eva Benckiser[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Lothastrasse 1, 47057 Duisburg, Germany — [3]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

A promising approach for the manipulation of quantum states involves the epitaxial stabilization of certain orbital occupations, i.e. orbital en-

gineering. Here we use resonant x-ray reflectometry to extract quantitative depth-dependent x-ray linear dichroism profiles of thin slabs of YVO_3 embedded in a superlattice with $LaAlO_3$. Our data reveal an artificial, layered orbital polarization, where the average occupation of xz and yz orbitals at the interface is inverted compared to the central layers of YVO_3. We attribute this effect to a combination of epitaxial strain and spatial confinement by $LaAlO_3$. Further, insights from *ab initio* calculations and scanning transmission electron microscopy indicate that the selection of a suitable spacer layer material, layer thickness of the transition metal oxide, facet of substrate, and sign of strain can together implement a desired orbital polarization pattern. Our study demonstrates the use of orbital engineering as a promising approach for the theory-guided rational design of quantum materials.

DS 15: 2D Materials 5 (joint session HL/CPP/DS)

Time: Wednesday 9:30–12:00 Location: H36

DS 15.1 Wed 9:30 H36

Dark exciton anti-funneling in monolayer transition metal dichalcogenides — •Roberto Rosati[1], Robert Schmidt[2], Samuel Brem[1], Raül Perea-Causín[3], Iris Niehues[4], Johannes Kern[2], Johann Adrian Preuss[2], Robert Schneider[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Ermin Malic[1,3] — [1]Philipps-Universität Marburg — [2]University of Münster — [3]Chalmers University of Technology — [4]CIC nanoGUNE BRTA

Current nanoelectronics relies on transport. While charged carriers can be controlled by electric fields, atomically thin semiconductors are governed by excitons, which are neutral electron-hole pairs. Recently, strain engineering has been introduced to manipulate exciton diffusion [1] and propagation [2] in monolayer transition metal dichalcogenides. Strain-induced energy gradients give rise to exciton funneling up to a micrometer range. Combining spatiotemporal photoluminescence measurements with microscopic theory, here we track the way of excitons in time, space and energy. Surprisingly we find that in WS_2 excitons move away from high-strain regions, contrary to what we observe in $MoSe_2$ [2]. This anti-funneling behavior can be ascribed to dark excitons, whose strain-induced energy variations are opposite compared to bright excitons. Our findings open new possibilities to control transport in exciton-dominated materials.

[1] R. Rosati et al., 2D Mater. 8, 015030 (2021).
[2] R. Rosati, R. Schmidt et al., Nat. Commun. 12, 7221 (2021).

DS 15.2 Wed 9:45 H36

Ultrafast nanoscopy of a Mott transition in twisted bilayer WSe_2 — •Svenja Nerreter[1], Thomas Siday[1], Fabian Sandner[1], Samuel Brem[2,3], Martin Zizlsperger[1], Felix Schiegl[1], Raul Perea-Causin[3], Markus Plankl[1], Philipp Merkl[1], Fabian Mooshammer[1,4], Markus A. Huber[1], Ermin Malic[2,3], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg — [2]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Physics, Chalmers University of Technology, 41296 Gothenburg, Sweden — [4]Department of Physics, Columbia University, New York, NY 10027, USA

The density-driven transition of an exciton gas into a Fermi liquid of unbound electron-hole pairs has formed a compelling testing ground of many-body physics. Layered transition metal dichalcogenides feature advantageous conditions, yet nanoscale inhomogeneities have complicated quantitative studies of this elusive transition. Here, we use ultrafast polarization nanoscopy to trace optically bright and dark electron-hole pairs during an exciton Mott transition in a twisted homobilayer of WSe_2. At elevated densities, initially monomolecular recombination dynamics of optically dark excitons continuously evolve into the bimolecular recombination of unbound electron-hole pairs. We directly reveal how the Mott transition varies over nanometer length scales, evidencing strong spatial disorder in stacked monolayers and demonstrating the capabilities of our technique to resolve the local interplay of strong electronic correlations.

DS 15.3 Wed 10:00 H36

Rashba excitons in the 2D Ruddlesden-Popper perovskite (BA)MAPI — •Philipp Moser[1], Martin Schalk[1], Atsuhiko Miyata[2], Joachim Wosnitza[2], Andreas Stier[1], and Jonathan Finley[1] — [1]Walter Schottky Institute, Garching, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Two-dimensional organic-inorganic perovskites have emerged as remarkable materials for energy conversion, optoelectronic and spintronic applications. Recently, the role of spin-orbit (SO) coupling and the resulting effects on the band-structure and dark/bright optical transitions has become a key topic of interest. The necessary structural inversion asymmetry for SO-coupling is predicted to stem from the organic cations comprising the crystals. As a result, dark excitons, red detuned from the bright exciton, have been discussed in this material system. Here, we investigate the exciton physics of the 2D Ruddlesden-Popper perovskite (BA)MAPI. By performing one-photon absorption, -PL and two-photon PLE spectroscopy, we investigate the optical transitions close to the R-point of the Brillouin zone and find distinct 2-photon transitions blue detuned from the ground state exciton that can be explained by a Rashba-split band-structure. Utilizing high-field magneto-spectroscopy up to B=60T, we determine that these absorption features are due to Wannier excitons. We determine the size and binding energy from the diamagnetic shift of the features and obtain evidence that 2D (BA)MAPI hosts strongly bound Rashba excitons.

DS 15.4 Wed 10:15 H36

Ultrafast pseudospin quantum beats in multilayer WSe2 and MoSe2 — •Simon Raiber[1], Paulo E. Faria Junior[2], Dennis Falter[1], Simon Feldl[1], Petter Marzena[1], Kenji Watanabe[3], Takashi Taniguchi[4], Jaroslav Fabian[2], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

We present investigations of excitonic transitions in mono- and multilayer WSe2 and MoSe2 materials by time-resolved Faraday ellipticity (TRFE) with in-plane magnetic fields, of up to B = 9 T. In monolayer samples, the measured TRFE time traces are almost independent of B, which confirms a close to zero in-plane exciton g factor, consistent with first-principles calculations. In stark contrast, we observe pronounced temporal oscillations in multilayer samples for B > 0. Remarkably, the extracted in-plane g factors are very close to reported out-of-plane exciton g factors of the materials, namely |g< 1s| = 3.1 +/- 0.2 and 2.5 +/- 0.2 for the 1s A excitons in WSe2 and MoSe2 multilayers, respectively. Our first-principles calculations nicely confirm the presence of a non-zero in-plane g for the multilayer samples. We propose that the oscillatory TRFE signal in the multilayer samples is caused by pseudospin quantum beats of excitons, which is a manifestation of spin- and pseudospin layer locking in the multilayer samples.

DS 15.5 Wed 10:30 H36

Nonlinear Exciton Dynamics in Layered Heterostructures — •Vipin Krishna[1], Xiao Chen[2], Tarlan Hamzayev[1], Silvana Botti[2], and Giancarlo Soavi[1] — [1]Institute of Solid state Physics,Friedrich-Schiller-University,Jena — [2]Institute of Theoretical Solid State Theory and Optics,Friedrich-Schiller-University,Jena

Transition-metal-dichalcogenides and related heterostructures(HS) are promising candidates for photonic and optoelectronic applications owing to strong light-matter coupling and electrically-tunable carrier dynamics.However,the presence of intense nonlinear effects such as Exciton-Exciton Annihilation(EEA)[1] limits the maximum realizable exciton-density,and is particularly efficient for interlayer-excitons(IL) due to their out-of-plane dipole nature[2].In this work,we systematically study the onset of EEA in type-II WS2/WSe2 HS by steady-state and nonlinear time-resolved PL.We infer that in HS the generation-rate is at least one order of magnitude larger for interlayer compared to intralayer-excitons for a given excitation-fluence, as expected from the ultrafast interlayer-charge-transfer and consequent IL formation.However,we do not observe stronger EEA for interlayer compared to intralayer-excitons and observe that for HS the recombination-

dynamics are identical for both,suggesting that the EEA mechanism is dominated by the total excitonic-density via intra and interlayer-exciton interactions.Our work provides new insights on EEA mechanism, which is of paramount importance for optoelectronic-devices and study of excitonic-condensates with layered-materials.[1]Kuechle et.Al.J.OMX(2021),12.[2]Sigl et.Al.Phys.Rev.B 105,035417.

15 min. break

DS 15.6 Wed 11:00 H36

Tunable exciton-polaritons emerging from WS_2 monolayer excitons in a photonic lattice at room temperature — •Lukas Lackner[1], Marco Dusel[2], Oleg Egorov[3], Bo Han[1], Heiko Knopf[3], Falk Eilenberger[3], Carlos Anton-Solanas[1], Sven Höfling[2], and Christian Schneider[1] — [1]University of Oldenburg, Oldenburg, Germany — [2]University of Würzburg, Würzburg, Germany — [3]Friedrich Schiller University Jena, Jena, Germany

The engineering of non-linear light-matter states in optical lattices has emerged as a key research strategy for the exploration of Hamiltonians in the spirit of ultrafast- and possibly quantum-simulation. It furthermore has revealed its potential to probe non-trivial topology phenomena. Excitons in atomically thin crystals have emerged as an ideal active medium for such purposes, since they couple strongly with light, and bear the potential to harness giant non-linearities and interactions.

In this work, we present an experiment conducted at room temperature in an open optical cavity of high quality, with an implemented one-dimensional photonic lattice. In our present work we integrate an atomically thin layer of WS_2 in such a device. We discuss the emergence and tunability of a lattice-band-structure in the tight-binding configuration at room temperature, fuelled by the emission from monolayer excitons[1].

References

[1] L. Lackner *et al., Nat Commun* **12**, 4933 (2021).

DS 15.7 Wed 11:15 H36

Optical Spectroscopy of Colloidal Transition Metal Dichalcogenides — •André Philipp Frauendorf[1], André Niebur[2], Jens Hübner[1], Jannika Lauth[2,3], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover — [3]Institut für Physikalische und Theoretische Chemie, Universität Tübingen

Atomically thin transition metal dichalcogenides (TMDs) are at the forefront of a new generation of two-dimensional semiconductor systems and experience an increasing research interest due to their unique optical properties. As an additional fabrication approach the wet-chemical synthesis has emerged as a promising method for the straightforward solution-processing of these materials. [1] Nevertheless, the optical properties of colloidal TMD mono- and few-layer structures have been sparsely studied.

Here, we demonstrate room-temperature micro-photoluminescence of colloidal TMD nanosheets. Both, mono-and multilayer photoluminescence are observed rendering these delicate structures fully competitive with conventionally fabricated TMDs. [1] In addition temperature-dependent transient absorption measurements are presented as a convincing technique for the exploration of the ultra-fast recombination dynamics of two-dimensional materials. [2]

[1] A. Frauendorf et al., J. Phys. Chem. C 125, 18841 (2021).
[2] A. Frauendorf et al., Manuscript in preparation (2022).

DS 15.8 Wed 11:30 H36

Capacitively and inductively coupled excitons in bilayer MoS_2 — •Lukas Sponfeldner[1], Nadine Leisgang[1], Shivangi Shree[2], Ioannis Paradisanos[2], Kenji Watanabe[3], Takashi Taniguchi[4], Cedric Robert[2], Delphine Lagarde[2], Andrea Balocchi[2], Xavier Marie[2], Iann C. Gerber[2], Bernhard Urbaszek[2], and Richard J. Warburton[1] — [1]Department of Physics, University of Basel — [2]Université de Toulouse, INSA-CNRS-UPS, LPCNO — [3]Research Center for Functional Materials, National Institute for Materials Science — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science

Exciton-exciton couplings in semiconductors lead to a plethora of phenomena such as nonlinear optical effects and quantum condensation. Transition-metal dichalcogenides constitute a versatile platform to study these effects as the excitons are very robust and their couplings can be controlled by exploiting their spin and valley properties.

Here, we probe exciton-exciton couplings in gated-homobilayer MoS_2. Using a driven-coupled oscillator model it is shown that the measured optical susceptibility reveals both the magnitude and the phase of the coupling constants. The interlayer excitons (IE) and intralayer B-excitons couple via a 0-phase (capacitive) coupling; the IE and the intralayer A-excitons couple via a π-phase (inductive) coupling. Using the IE as a sensor, the A-B intravalley exchange coupling is determined, a result which is also relevant for a monolayer. Finally, we realize a bright and highly tunable lowest-energy momentum-direct exciton at high electric fields.

DS 15.9 Wed 11:45 H36

Controlling the non-linearity in two dimensional materials — •Mathias Federolf and Sven Höfling — Technische Physik, Universität Würzburg, 97074 Würzburg, Germany

Recently Datta et al. [1] have shown that exciton-polaritons in bilayer MoS_2 experience a blueshift due to interacting with other exciton-polaritons. The observed blueshift is non-linear with respect to the laser power used for excitation. Due to the bilayer's nature interlayer-excitons can occur, which exhibit an out of plane dipole moment. Using an electric field along the out of plane axis those dipoles can be aligned and used to influence the exciton-exciton interaction. By using a varying electric field, we map the parameter space to gain deterministic control over the blueshift. Understanding and controlling the system allows us to tune the polariton-polariton interaction such that they can be used in future application i.e., single-photon sources.

[1] Datta, Biswajit, et al. arXiv preprint arXiv:2110.13326 (2021).

DS 16: Thin Film Applications 2

Time: Wednesday 11:00–12:00 Location: H14

DS 16.1 Wed 11:00 H14

High Open-Circuit Voltage $Cs_2AgBiBr_6$ Carbon-Based Perovskite Solar Cells Via Green Processing of Ultrasonic Spray-Coated Carbon Electrodes from Waste Tire Sources — •Fabian Schmitz and Teresa Gatti — Center for Materials Research, Justus Liebig University, Giessen, Germany

Although top-notch lead-based perovskite solar cells (PSCs) achieve power conversion efficiencies >25%, they are still hindered from commercial implementation by their low environmental stability, high toxicity and optimizable costs. The latter could be reduced by eliminating the metal back electrode as well as the hole-transport material by substituting both with a conductive carbon material to create carbon-based PSCs (C-PSCs). Furthermore, the utilization of perovskite materials based on other metallic compounds could tackle the other two issues of stability and toxicity. A promising example that combines both high environmental stability and low toxicity is the double perovskite $Cs_2AgBiBr_6$.

In our work, we present the deposition of "green" carbon electrodes onto $Cs_2AgBiBr_6$ thin films via high-throughput ultrasonic spray coating to prepare lead-free C-PSCs. For our sustainable approach, we started from a carbon material obtained from the hydrothermal recycling of waste tires and dispersed it in isopropanol. This additive-free ink worked as a precursor for the upscalable ultrasonic spray deposition method to fabricate carbon electrodes under ambient atmosphere and at a low substrate temperature. Through this procedure we obtained C-PSCs with record open-circuit voltages of >1.2 V.

DS 16.2 Wed 11:15 H14

Indirect band gap semiconductors for thin-film photovoltaics: High-throughput calculation of phonon-assisted absorption — •Jiban Kangsabanik, Mark Kamper Svendsen, Alireza Taghizadeh, and Kristian S. Thygesen — Technical University of Denmark, Denmark

Photovoltaics is one of the most promising ways towards meeting the ever-increasing global energy demand in a sustainable and eco-friendly way. Thin-film materials (GaAs, CdTe, InP, CIGS, $MAPbI_3$, etc) are rapidly growing in terms of market share in recent times, showing comparable efficiencies to the current Si-based technology. Currently, these well-known thin-film materials possess some major drawbacks associated with low material abundance (In, Ga), toxicity (Cd, As, Pb), and long-term device stability (perovskites). As such, finding new materials with desirable physical attributes remains one of the key aspects in this area. Indirect bandgap semiconductors, which occupy a major portion of the semiconductor space are mostly ignored in recent material screening studies. Here, we propose a recipe to evaluate PV efficiency for indirect gap materials via calculating phonon-assisted absorption, which is high-throughput friendly. Using this recipe, we evaluate chemically stable unary and binary materials from the Open Quantum Materials Database for PV application. From our final screening, we identify well-known binary thin film materials (GaAs, CdTe, and InP) as well as a number of the emerging PV materials (PbS, SnS, Se, GeSe, etc). Additionally, we find a number of indirect gap materials with potential for thin-film PV device application.

DS 16.3 Wed 11:30 H14

Physical unclonable function based on unsorted carbon nanotube random networks in multi-contact field-effect transistors — Jonas Schroeder[1], •James W. Borchert[1], Patrick Schuster[2], Peter Eder[2], Stefan Heiserer[3], Josef Biba[3], Georg S. Duesberg[3], Ulrich Rührmair[2,4], and R. Thomas Weitz[1] — [1]Georg-August Universität Göttingen, Göttingen, Germany — [2]Ludwig-Maximilians-Universität München, München, Germany — [3]Universität der Bundeswehr München, Neubiberg, Germany — [4]University of Connecticut, Storrs CT 06269, USA

The standard practice in cryptography of using digital binary keys that are permanently stored on devices is prohibitively inefficient for some applications and open to both physical and software-based attacks. A promising alternative approach known as 'physical unclonable function' (PUF) instead uses the inherent random variation in fabrication to create physical 'keys' that produce unique randomized responses to defined challenges. Electrical PUF devices based on random networks of unsorted carbon nanotubes (CNTs) have shown promise, but so far have been limited in terms of scaling up the number of challenge-response pairs (CRPs) that can be extracted. Here, we demonstrate how gating the CNT networks might be a useful method for expanding the number of CRPs, thus strengthening the scalability of the PUF. We show CNT networks implemented in modified field-effect transistors with up to 12 contacts. The output randomness and stability of the devices are investigated, and further routes for improvement are discussed.

DS 16.4 Wed 11:45 H14

Redox-based Memristive Devices for Neuromorphic Systems — •Benjamin Spetzler, Seongae Park, Anna Linkenheil, Tzvetan Ivanov, and Martin Ziegler — Technical University Ilmenau, Ilmenau, Germany

Redox-based memristive devices have demonstrated promising properties for their application as synaptic elements in neuromorphic computing systems. The device characteristics are the product of a variety of complex mechanisms, and electronic and ionic processes need to be precisely tuned, which requires a deep understanding of the underlying physical mechanisms and control of the fabrication parameters. We present redox-based memristive elements and show how their properties can be tailored by systematic design variations for applications in neuromorphic computing architectures. In this context, the influence of different oxide layer systems and electrode materials on the device characteristics is analyzed to assess their properties for neuromorphic computing. The experimental findings are supported by a numerical device model, which connects the physical processes with technology parameters, and permits a deeper understanding of the origin of the current-voltage hysteresis. Furthermore, we discuss the system integration of memristive devices and present memristive device arrays.

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

DS 17: 2D Materials 6 (joint session DS/CPP)

Time: Wednesday 11:15–13:00 Location: H17

DS 17.1 Wed 11:15 H17

Curvature-induced spin-orbit splitting in transition metal dichalcogenide nanotubes and wrinkles — Mohammadreza Daqiqshirazi and •Thomas Brumme — Theoretical Chemistry, TU Dresden

Strain engineering provides a powerful means to tune the properties of 2D materials. Homogeneous strain fields have been studied extensively, and there are standard techniques for altering properties of 2D materials even in industry. On the other hand, much less is known about how inhomogeneous strain affects the electronic properties of 2D materials. We employed DFT to understand the correlation between the atomic and the electronic structure in nanoscale wrinkles and nanotubes of the prototypical transition metal dichalcogenide WSe_2. Our research shows that the symmetry breaking in these structures lead to strong Rashba-like spin-orbit splitting of the bands at the Γ point and that they thus may be utilized in future tunable spintronics devices.

DS 17.2 Wed 11:30 H17

Moiré-Bose-Hubbard model for interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Niclas Götting, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Bremen

Introducing a twist between two superimposed TMD monolayers results in a new superlattice whose properties heavily depend on the twist angle. These so-called moiré structures of TMD materials like MoS_2/WS_2 can host interlayer excitons (IXs) which perceive the varying atomic registry over the moiré unit cell as an effective moiré potential. In such structures, correlated states can emerge, in which the IXs are strongly localized to the potential minima due to exciton-exciton interactions.

We investigate the phases of these trapped moiré IXs by approximating them as bosonic particles and mapping the system onto a Bose-Hubbard model [1]. Our methods allow us to calculate the hopping and two-particle interaction terms of the Bose-Hubbard model for n-th nearest neighbors. To examine the strong impact of dielectrics surrounding the heterobilayer, we introduce a Keldysh potential to the calculation and thereby obtain first results of the twist-angle dependent phases of moiré IXs in twisted TMD heterobilayers.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

DS 17.3 Wed 11:45 H17

Enhanced Potassium Storage Capability of Two-Dimensional Transition-Metal Chalcogenides — •Vincent Hartmann and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Potassium-ion batteries (PIBs) have been considered a promising alternative to lithium-ion batteries due to their merits of high safety and low cost. Two-dimensional transition metal chalcogenides (2D TMCs) with high theoretical specific capacities and unique layered structures have been proven to be amenable materials for PIB anodes. However, some intrinsic properties including severe stacking and unsatisfactory conductivity restrict their electrochemical performance, especially rate capability. Herein, a heterostructure of high-crystallized ultrathin MoSe2 nanosheet-coated multiwall carbon nanotubes was prepared and its electrochemical properties were investigated. In such a heterostructure, the constructive contribution of CNTs not only suppresses the restacking of MoSe2 nanosheets but also accelerates electron transport. Meanwhile, the MoSe2 nanosheets loaded on CNTs exhibit an ultrathin feature, which can expose abundant active sites for the electrochemical reaction and shorten the K+ diffusion length. Therefore, the synergistic effect between ultrathin MoSe2 and CNTs endows the resulting nanocomposite with superior structural and electrochemical properties. Additionally, the high crystallinity of the MoSe2 nanosheets further leads to the improvement of electrochemical performance.

DS 17.4 Wed 12:00 H17

Single photon emission of quantum emitters in WSe2 monolayers and their temperature-dependent coherence properties — •Martin von Helversen[1], Paul Schlaugat[1], Chirag Palekar[1], Carlos Antón-Solanas[2], Bárbara Rosa[1], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institute for solid state physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute for Physics, Carl von Ossietzky Universtität Oldenburg, 26111 Oldenburg, Germany

Two-dimensional van der Waals monolayers have appeared as novel type of semiconducting materials, which provide a platform for the exploration of their highly interesting optical, electronic and structural properties. Within the transition-metal dichalcogenides, WSe2 has turned out to be the most promising platform for two-level single-photon emitters, generated either by applied strain to the monolayer-flake [1,2], or by defects in the material [2]. However, the quality of the generated photons still lacks behind other systems as for example semiconductor quantum dots. In this work, we study single emitters of a strained WSe2-monolayer showing linewidths around 100 μeV at 4 K. In quasi-resonant pulsed optical excitation a second-order autocorrelation value down to $g^{(2)}(0)=0.037(5)$ is measured. We further study their temperature dependent first-order coherence properties via a scanning Michelson interferometer, which yields coherence times up to 48 ps.

[1] L. N. Tripathi et al., ACS Photonics 5, 1919 (2018)
[2] K. Parto et al., Nat. Commun. 12, 3585 (2021)

DS 17.5 Wed 12:15 H17

Spin-defect characteristics of single sulfur vacancies in monolayer MoS_2 — •Alexander Hötger[1], Tomer Amit[2], Julian Klein[3], Katja Barthelmi[1], Thomas Pelini[4], Alex Delhomme[4], Sergio Rey[5], Marek Potemski[4,6], Clément Faugeras[4], Galit Cohen[2], Daniel Hernangómez-Pérez[2], Takashi Taniguchi[7], Kenji Watanabe[7], Christoph Kastl[1], Jonathan Finley[1], Sivan Refaely-Abramson[2], Alexander Holleitner[1], and Andreas Stier[1] — [1]Walter Schottky Institute, Garching, Germany — [2]Weizmann Institute of Science, Rehovot, Israel — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Laboratoire National des Champs Magnetiques Intenses, Grenoble, France — [5]Technical University of Denmark, Lyngby, Denmark — [6]University of Warsaw, Warszawa, Poland — [7]National Institute for Materials Science, Tsukuba, Japan

Single spin defects in 2D transition-metal dichalcogenides are natural spin-photon interfaces for quantum applications. Here we report high-field magneto-spectroscopy from three emission lines of He-ion induced sulfur vacancies in monolayer MoS_2. The distinct valley-Zeeman splitting and the brightening of dark states necessitates spin-valley selectivity of the defect states and lifted spin-degeneracy at zero field. Comparing our results to ab-initio calculations identifies the nature of the defect luminescence. Analysis of the optical degree of circular polarization reveals that the Fermi level is a parameter that enables the tunability of the emitter. These results show that defects in 2D semiconductors may be utilized for quantum technologies.

DS 17.6 Wed 12:30 H17

Probing excitonic population dynamics by nonlinear optical wave mixing in monolayer WSe2 — •Jonas M. Bauer, Lijue Chen, Philipp Wilhelm, Sebastian Bange, John M. Lupton, and Kai-Qiang Lin — Department of Physics, University of Regensburg, 93053 Regensburg, Germany

Monolayer semiconductors are emerging platforms for strong nonlinear light-matter interaction, due to their giant oscillator strength of tightly bound excitons. Recently, we reported the existence of a new excitonic species, the high-lying exciton (HX), in monolayer WSe2. The HX appears at around twice the energy of the band-edge A-exciton, forming a ladder-type excitonic three-level system. We demonstrate excitonic quantum interference in monolayers [1] and twisted bilayers [2]. Here, we apply time-resolved nonlinear spectroscopy to probe the excitonic dynamics. We find that a significant time difference between two light pulses is necessary for optimal sum-frequency generation (SFG) and four-wave mixing (FWM) if one of the pulses is in resonance with an excitonic transition. The experimental results are rationalized by numerical calculations based on a density-matrix approach and provide insights into coherent exciton dynamics on a femtosecond scale.

[1] K.-Q. Lin, S. Bange, & J. M. Lupton, Nat. Phys. 15, 242-246 (2019).
[2] K.-Q. Lin, J.M. Bauer et al., Nat. Commun. 12, 1553 (2021).

DS 17.7 Wed 12:45 H17

Characterization of 2D WSe2 by high-resolution STEM and Differential Phase Contrast STEM — •Maja Groll[1], Julius Bürger[1], Ioannis Caltzidis[2], Marc Sartison[2], Klaus Jöns[2], and Jörg Lindner[1] — [1]Nanostructuring, Nanoanalysis and Photonic Materials Group, Department of Physics, Paderborn University, Germany — [2]Hybrid Quantum Photonic Devices, Department of Physics, Paderborn University, Germany

2D transition metal dichalcogenides (TMDs) are gaining attention as their optical and electronic properties differ from those of their bulk counterparts. In particular, layer thickness-dependent properties, such as the transition from an indirect to a direct band gap in monolayers, make these materials interesting for photonic and optoelectronic applications. At the same time 2D-TMDs are ideal materials for the advancement of new techniques in scanning transmission electron microscopy (STEM) like differential phase contrast (DPC)-STEM. Using a spherical aberration corrected STEM, this technique enables the quantification of atomic electric fields with sub-atomic resolution if the specimen is sufficiently thin. In order to examine the atomic electric fields of TMDs, we transferred mechanically exfoliated mono- and multilayers of tungsten diselenide (WSe2) to TEM grids. The atomic structure of WSe2 flakes and their thickness are studied using TEM, energy filtered TEM and STEM. STEM-DPC measurements are performed using an eight-fold segmented bright-field STEM detector measuring the beam deflection due to the internal fields. Results are presented for WSe2 flakes of different thickness and compared with simulations.

DS 18: Thin Oxides and Oxide Layers 1

Time: Wednesday 15:00–16:00 Location: H14

DS 18.1 Wed 15:00 H14

Simulation analysis of sneak paths effect in the memristor-based crossbar topology — •Ziang Chen[1,2,3], Hao Cai[1,2,3], Christopher Bengel[4], Feng Liu[5], Xianyue Zhao[1,2,3], Heidemarie Schmidt[1,2], Stephan Menzel[5], and Nan Du[1,2,3] — [1]1)*FSUJena, Jena, Germany — [2]2)*IPHT, Jena, Germany — [3]3)*TU Chemnitz, Chemnitz, Germany — [4]4)*RWTH Aachen, Aachen, Germany — [5]5)*FZJ, Juelich, Germany

The high demand for performance and energy efficiency poses challenges for computing systems. The memristor-based crossbar architecture is enthusiastically regarded as a potential competitor to traditional solutions. Nonetheless, due to the lack of a switching control per cell, the memristor-based crossbar architecture suffers from the sneak paths that limit the range of accurate operation of the crossbar array. In this talk, the memristor-based passive crossbar geometry is studied and different topological patterns-one word line pull-up (OneWLPU) and all word line pull-up (AllWLPU)-is presented. In the worst-case scenario of two crossbar topological patterns, the read margin is defined as an accurate estimation for the sneak paths effects. For suppressing the sneak paths effects, in the Cadence simulation of two crossbar topological patterns based on the mathematical memristor model, the relevance between the read margin and other functional elements in the crossbar topology, i.e. pull-up resistance, line resistance, On/Off ratio, is revealed and analyzed. This work offers a beneficial reference and feasible solutions for the future optimization of crossbar topology with the intention of diminishing sneak paths effects.

DS 18.2 Wed 15:15 H14

Mapping the local strain distribution of oxide membranes using polarization-dependent micro-Raman spectroscopy — •Matthias T. Elm, Alexander Konetschny, Marcel Weinhold, Christian Heiliger, and Peter J. Klar — Justus-Liebig University, Gießen, Germany

Free-standing ceramic membranes are of great interest for miniaturized

electrochemical devices, such as micro-solid oxide fuel cells, sensors or memory devices. Free-standing membranes exhibit residual strain, which alters the electrical conductivity and, thus, the performance of the device. Detailed knowledge of the local strain distribution in the membrane is therefore of paramount importance. Here, we show that the local strain state of the membrane can be monitored using polarization dependent micro-Raman mapping. Due to the residual strain the triply degenerate F_{2g} mode splits and the contribution of their Raman intensity to the overall Raman signal depends on the measurement geometry and the polarization of the incoming and scattered light. Varying the polarization of the incoming excitation light results in different averaging of the Raman-active modes. These results clearly demonstrate that polarization-dependent Raman measurements have the potential to yield additional insight into the local strain distribution in free-standing oxide membranes.

DS 18.3 Wed 15:30 H14

Soft RIXS study of alumina-titania thin films heterostructure to reveal the nature of 2-dimensional electron system — •Deok-Yong Cho — Department of Physics, Jeonbuk National University, South Korea

Al2O3/TiO2 binary oxide heterostructure is a novel 2-dimensional electron system (2DES) compatible with mass production. The electronic structure of the 2DES was examined using resonant inelastic soft X-ray scattering. The TiO2 thickness-dependent evolution in the Ti L3-edge energy loss features unequivocally evidenced the presence of Ti3+ state at the interface and a substantial electron-phonon coupling effects. This suggests that the 2DES properties can be controlled via well-established TiO2 engineering so that the binary oxide heterostructure would be a promising candidate for 2DES-based device application.

This work was done in collaboration with Yu-Cheng Shao, Cheng-Tai Kuo, Xuefei Feng and Yi-De Chuang (Advanced Light Source, USA), and Tae Jun Seok, Ji Hyeon Choi and Tae Joo Park (Hanyang University, South Korea). DOI: 10.1002/adfm.202104430

DS 18.4 Wed 15:45 H14

Tuning the electrochemical properties of multifunctional CoO_x catalyst layers by plasma-enhanced atomic layer deposition — •Matthias Kuhl, Gabriel Grötzner, Laura Wagner, Alex Henning, Ian Sharp, and Johanna Eichhorn — Walter Schottky Institute, Technical University of Munich, Munich, Germany

Artificial photosynthetic systems are often limited by the poor efficiency and material instability of photoelectrodes under harsh PEC conditions. One strategy towards stable and efficient systems is to interface the semiconductor light absorber with conformal and ultrathin catalytic layers, which still permit interfacial charge transport and minimize losses due to parasitic light absorption. In this context, conformal, biphasic $Co_3O_4/Co(OH)_2$ catalyst layers were fabricated by means of plasma-enhanced atomic layer deposition (PE-ALD), which are simultaneously robust and electrochemically active. The nanocrystalline Co_3O_4 layer forms a durable interface to the substrate and the disordered $Co(OH)_2$ surface layer significantly improves the electrocatalytic oxygen evolution reaction activity. Here, we show that nonsaturated oxidation reactions can be applied to tune catalytic activity, chemical stability, and physical properties of the PE-ALD layer by leveraging low plasma exposure time and low plasma power. Based on these insights, the CoO_x films are interfaced with polycrystalline semiconductor thin films to generate highly stable and efficient multilayer photoelectrode assemblies. Overall, this work highlights the use of PE-ALD as a promising approach for engineering catalyst/semiconductor interfaces to create efficient and stable photoelectrodes.

DS 19: 2D Materials 7 (joint session DS/CPP)

Time: Wednesday 15:00–16:00 Location: H17

DS 19.1 Wed 15:00 H17

Gate-Tunable Helical Currents in Commensurate Topological Insulator/Graphene Heterostructures — •Jonas Kiemle[1,2], Lukas Powalla[3,4], Katharina Polyudov[3,4], Lovish Gulati[3], Maanwinder Singh[1,2], Alexander Holleitner[1,2], Marko Burghard[3,4], and Christoph Kastl[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Garching, Germany — [2]MCQST, München, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Van der Waals heterostructures made from graphene and three-dimensional topological insulators promise very high electron mobilities, a non-trivial spin texture and a gate-tunability of electronic properties. Here, we explore epitaxially grown interfaces between graphene and the lattice-matched topological insulator Bi_2Te_2Se. For this heterostructure, spin-orbit coupling proximity has been predicted to impart an anisotropic and electronically tunable spin texture. Polarization-resolved second-harmonic generation, Raman spectroscopy, and time-resolved magneto-optic Kerr microscopies are combined to demonstrate that the atomic interfaces align in a commensurate symmetry with characteristic interlayer vibrations. By polarization-resolved photocurrent measurements, we find a circular photogalvanic effect which is drastically enhanced at the Dirac point of the proximitized graphene. We attribute the peculiar gate-tunability to the proximity-induced interfacial spin structure.

DS 19.2 Wed 15:15 H17

Topological Invariant of Acoustic Phonons in 2D materials — •Gunnar Lange[1], Adrien Bouhon[1], Bartomeu Monserrat[1,2], and Robert-Jan Slager[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Materials Science and Metallurgy, University of Cambridge, UK

2D materials that live in a 3D space display an unusual acoustic phonon mode: the flexural mode. This mode disperses quadratically away from the center of the acoustic Brillouin zone, and corresponds to a flexing of the material out-of-plane. This differs markedly from the linear dispersion displayed by the in-plane modes, and leads to an unusual triple degeneracy at the zone center. This triple degeneracy is enforced by the Nambu-Goldstone theorem, rather than symmetry, as will be discussed. Such band degeneracies frequently have associated topological invariants. For this triple degeneracy, the topological invariant turns out to generically be of quaternionic type (Euler topology), but reduces to a $\mathbb{Z}_2$ invariant under fairly general assumptions. The invariant has important implications for 2D materials grown on a substrate, as it dictates how the bands are split due to the presence of the substrate. This will be discussed in the context of graphene, where the $\mathbb{Z}_2$ invariant turns out to be non-trivial.

This talk is based on: Lange, G. F., Bouhon, A., Monserrat, B., and Slager, R.-J., "Topological continuum charges of acoustic phonons in two dimensions and the Nambu-Goldstone theorem" Phys. Rev. B **105**, 064301 (2022)

DS 19.3 Wed 15:30 H17

Coupled Bilayer Graphene Quantum Dots — •Angelika Knothe[1,2] and Vladimir Fal'ko[2,3] — [1]Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]National Graphene Institute, University of Manchester, Manchester, UK — [3]Henry Royce Institute for Advanced Materials, University of Manchester, Manchester, UK

Bilayer graphene quantum dots are promising for spin and valley qubits [1,2,3]. A functional quantum information architecture requires scalable multi-qubit systems. We theoretically study electrostatically confined double-dots and few-dot arrays in bilayer graphene. We quantify the inter-dot couplings for different dot parameters such as the field-induced gap, the confinement shape, and the inter-dot distance. This dependence on external parameters allows tuning the dot arrays into different regimes for which we study the extended Hubbard Hamiltonians and identify the spin and valley level structure. Our results will help to advance the use of bilayer graphene quantum dots for quantum technologies.

[1] A. Knothe, L. I. Glazman, V. Fal'ko, New Journal of Physics 24 (4), 043003 (2022)

[2] S. Möller, L. Banszerus, A. Knothe, C. Steiner, E. Icking, S. Trellenkamp, F. Lentz, K. Watanabe, T. Taniguchi, L. Glazman, V. Fal'ko, C. Volk, C. Stampfer, Phys. Rev. Lett. 127, 256802 (2021)

[3] A. Knothe, V. Fal'ko, Phys. Rev. B 101, 235423 (2020)

DS 19.4 Wed 15:45 H17

Electron cavity optics in bilayer graphene — Lukas Seemann[1], •Angelika Knothe[1], Klaus Richter[2], and Martina Hentschel[1] — [1]Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Rapid developments in the field of 2D materials and their nanostructures make it possible to trap charge carriers with different dispersions in various confinement geometries with a high degree of control. This progress now allows studying 2D electron optics phenomena enriched by the charge carriers' different electronic and topological properties compared to the photonic case. Here, we theoretically investigate cavities in gapped bilayer graphene employing an approach based on ray-wave correspondence [1]. We identify the influence of the materials' trigonally warped band structure [2] on the fermion optics characteristics that we show to be conveniently tuneable by gate voltages. Similar considerations can be applied to electron optics in other 2D materials.

[1] J.-K. Schrepfer, S. Chen, M.-H. Liu, K. Richter, and M. Hentschel, Phys. Rev. B 104, 155436 (2021)

[2] C. Gold, A. Knothe, A. Kurzmann, A. Garcia-Ruiz, K. Watanabe, T. Taniguchi, V. Fal'ko, K. Ensslin, T. Ihn, Phys. Rev. Lett. 127, 046801 (2021)

DS 20: Poster

Time: Wednesday 16:00–18:00 Location: P3

DS 20.1 Wed 16:00 P3

Thickness effect on ferroelectric domain formation in compressively strained K0.65Na0.35NbO3 epitaxial films — •Yankun Wang[1,2], Saud Bin Anooz[1], Gang Niu[2], Martin Schmidbauer[1], Lingyan Wang[2], Wei Ren[2], and Jutta Schwarzkopf[1] — [1]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — [2]Electronic Materials Research Laboratory, Xi'an Jiaotong University, Xi'an, China

Ferroelectrics are of increasing interest for a broad range of applications such as nonvolatile memory devices, transducers and MEMS sensors. Herein, the influence of thickness in epitaxial K0.65Na0.35NbO3 ferroelectric thin films grown on (110) TbScO3 substrate is systematically studied. By combining piezoresponse force microscopy and high-resolution x-ray diffraction, the occurrence of 90° stripe domains was demonstrated for the films with a thickness above 11 nm, while the domain periodicity is in good agreement with Kittel*s law. Furthermore, up to a thickness of 93 nm, elastic strain relaxation induced by the formation of ferroelectric domains is observed, whereas plastic strain relaxation plays only a minor role. With increasing film thickness three successive phases of ferroelectric domains were observed: i) Irregularly arranged orthorhombic c domains in the thinnest film, ii) periodically arranged 90° monoclinic MC domains up to a thickness of 25 nm and iii) flux closure vortex-like structure in thicker films to achieve the lowest equilibrium energy. These results demonstrate the importance of understanding the lattice relaxation mechanisms for intentional tuning of ferroelectric thin film properties.

DS 20.2 Wed 16:00 P3

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

Spin crossover (SCO) molecules are a promising type of material that can undergo reversible switching between low-spin (LS)- and high-spin (HS)-states upon external stimuli (heat, light, pressure, etc.)[1], making them useful for information technology, data storage and optoelectronics[2]. However, most SCO molecules need to be cooled significantly for this transition to be observable. We have investigated the hitherto unknown electronic structure of the complex molecule bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(II) ([Fe(HB(tz)3)2])[3] capable of above-RT transition by XPS and XAS measurements, since the distinct electronic structure in both spin-states unmistakably prove the transition between them.

[1]P. Gütlich and H. A. Goodwin. "Spin Crossover in Transition Metal Compounds I." Springer Berlin Heidelberg, May 2004. 356 pp. [2]E. P. Geest et al.,"Contactless Spin Switch Sensing by Chemo*Electric Gating of graphene". In: Advanced Materials (2020), p. 1903575. [3]S. Rat et al.,"Solvatomorphism and structural-spin crossover property relationship in bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(ii)". In: CrystEngComm 19.24 (2017).

DS 20.3 Wed 16:00 P3

Insights into the evaporation behaviour of FAI: material degradation and consequences for perovskite solar cells — Martin Kroll[1], Seren Dilara Öz[3], Zongbao Zhang[1], Ran Ji[1], •Tim Schramm[1,2], Tobias Antrack[1], Yana Vaynzof[1,2], Selina Olthof[3], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, IAPP — [2]Center for Advancing Electronics Dresden, CFAED — [3]Department of Chemistry, University of Cologne

Thermal co-evaporation is a promising method for large-scale uniform perovskite deposition. In this work, we look at the decomposition of formamidinium iodide (FAI) upon evaporation in high vacuum by tracking the composition of the residual gas with a mass spectrometer. We find that the precursor material degrades during the evaporation process into hydrogen cyanide (HCN) and sym-triazine (C3H3N3), leading to an increase in pressure, which is commonly observed during the deposition of FAI. Using optical characterization as well as x-ray photoelectron spectroscopy on co-deposited perovskite films, we demonstrate that this background pressure strongly affects the resulting film*s stoichiometry. Using two different vacuum setups, we are able to show that significant changes are imposed, e.g. on the optimized co-evaporation rates, by the specific vacuum chamber setup. Our results have important implications for the optimized evaporation of FA-based perovskites as they identify key issues related to the deposition of the FAI precursor.

DS 20.4 Wed 16:00 P3

In situ surface X-ray diffraction studies at high temperatures of Co oxide model catalysts for electrochemical water splitting — •Carl Hendric Scharf[1], Canrong Qiu[1], Jochim Stettner[1], Olvido Irrazábal-Moreda[2], Mathilde Bouvier[3], Fouad Maroun[3], and Olaf Magnussen[1] — [1]Institute of Experimental and Applied Physics, Kiel, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [3]Physique de la Matière Condensée, Ecole Polytechnique, Palaiseau, France

The development of low-cost electrocatalysts for electrochemical water splitting is of great interest for hydrogen technology. Among the best precious-metal-free electrode materials for the anodic oxygen evolution reaction (OER) in alkaline electrolysis are Co oxides such as Co_3O_4 and CoOOH. It was shown previously that a sub-nm thick $CoO_x(OH)_y$ skin layer is formed in the pre-OER potential range, which forms the active phase during OER. Furthermore, reversible and irreversible structural changes in the oxide bulk were detected in the pre-OER regime. So far the vast majority of publications on Co oxide OER electrolysis have been performed at room temperature. We present first results up to 60°C (typ. operating temperatures of commercial electrolysers). Using operando surface X-ray diffraction Co_3O_4 and CoOOH epitaxial films electrodeposited on Au(111) were studied in 0.1M NaOH at Petra III, Desy. These data are correlated with the electrochemical properties, determined by Cyclic Voltammetry and Optical Reflectivity, in order to provide insights into the temperature-dependence of skin layer thickness, bulk lattice changes and the stability of the oxides.

DS 20.5 Wed 16:00 P3

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

Cobalt monoxide, CoO, is an antiferromagnet (AF) with a Néel temperature of 293K. It is utilised to pin the magnetisation of Co layers via exchange bias and is employed in magnetic heterostructures. The interaction between ferromagnet (F) and AF layers is predicted to generate long-range spin-triplet superconductivity in F-S-AF heterostructures

[1]. CoO is a good candidate for the AF due to its strong magnetism, stability and low Neel temperature, which facilitates in-field cooling through the transition, improving magnetic uniformity. For the most part, CoO is synthesized by the oxidation of Co thin films. A fundamental understanding of how the Co phase (fcc or hcp) and oxidation environment influence the crystalline quality and surface morphology of the resultant CoO is lacking. In this work, we investigate the crystalline quality of the CoO as a function of Co phase and oxidation environment. As a second step towards a F-S-AF heterostructure, we also investigate the superconducting properties of superconducting Nb grown on the different CoO films. The properties of the niobium - especially at low thickness relevant to heterostructures - will, in theory, be influenced by the CoO magnetic and surface structure. 1. L. G. Johnsen et al., Phys. Rev. B, 103, L060505 (2021).

DS 20.6 Wed 16:00 P3

Pseudo-2-dimensional Ga_2O_3 structures grown on Al_2O_3 using metal-oxide catalyzed epitaxy (MOCATAXY) — •Justin Andreas Bich[1], Marco Schowalter[1], Tjark Liestmann[1], Sushma Raghuvansy[1], Jonathan McCandless[2], Manuel Alonso-Orts[1], Andreas Rosenauer[1], Martin Eickhoff[1], and Patrick Vogt[1] — [1]Institute of Solid-State Physics, Bremen University, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]School of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853, USA

Ga_2O_3 has attracted attention as a new wide-bandgap semiconductor—which can be alloyed with Al_2O_3—for high-power applications. However, the growth of group-III sesquioxides by molecular-beam epitaxy differs substantially from other material systems, e.g., III-V materials.

In this work, we present the growth of ultra-thin α-Ga_2O_3 (0001) on α-Al_2O_3 (0001) in a controlled self-passivating manner. Using MOCATAXY, we observe the formation of this 'pseudo' 2-dimensional (2D) α-Ga_2O_3 thin film and its growth passivation after reaching 2 nm thickness. This α-Ga_2O_3 2D thin film serves as a template for growing α-Ga_2O_3/α-Al_2O_3 quantum wells.

We present reflection-high energy electron diffraction, x-ray photoelectron spectroscopy, atomic force microscopy, x-ray diffraction, x-ray reflectivity, and transmission electron microscopy data, showing the existence and characteristics of this 'pseudo' 2D α-Ga_2O_3 thin film grown by MOCATAXY, and explain our results using a kinetic and thermodynamic framework.

DS 20.7 Wed 16:00 P3

An unconventional octahedral metal: AgSnTe2 — •Sophia Wahl, Christian Teichrib, Carl-Friedrich Schön, Maria Häser, Yuan Yu, and Matthias Wuttig — 1. Institute of Physics (Ia), RWTH Aachen University, Aachen, Germany

Phase-change materials (PCMs) provide a unique combination of properties. Switching from the amorphous to crystalline structural phase, their optical and electrical properties change significantly. While conventional PCMs undergo a change from covalent to metavalent bonding upon crystallization accompanied by a dielectric behavior in both phases [1], we observe a change from dielectric to metallic in the optical and electrical properties for the unconventional metal AgSnTe2 (AST).

We analyze the dielectric properties of amorphous and crystalline AST samples by employing optical spectroscopy from the infrared to UV/Vis range. Through a Kramers-Kronig analysis of the data, we can separate the contributions of the optical functions accordingly and yield insight into the nature of bonding. Transport measurements and the investigation of bond rupture in atom probe tomography support the findings and all imply a non-conventional bonding mechanism in crystalline AST.

This work is aiming to define a whole set of new plasmonic PCMs which are all located in one region of the materials bonding map[2].

[1] Wuttig et al., Nat. Photonics, 11, 2017

[2] Raty et al., Adv. Mater., 31, 2019

DS 20.8 Wed 16:00 P3

Structural and electronic investigations of Bismuth multilayers with DFT — •Fabian Teichert[1], Chitran Ghosal[1], Uwe Gerstmann[2], Christoph Tegenkamp[1], and Angela Thränhardt[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Department of Physics, Paderborn University, Paderborn, Germany

Bismuth shows a variety of interesting properties as bulk material but also as thin film, e.g. it is a topological insulator, shows strong spin-orbit coupling effects and has a semimetal-semiconductor transition concerning film thickness. The focus of this presentation will be on density functional theory (DFT) calculations, which have been done for Bi(110) multilayers to get insights into the concrete structure and electronic states. We compare the results with Bi multilayers, which have been grown epitaxially on graphene substrate and where (110) slabs have been figured out. They are treated with scanning tunneling microscopy (STM) measurements for various slab thicknesses. We found an even/odd scheme concerning the number of monolayers as well as concerning the number of bilayers indicating a structural relaxation like the black phosphorus allotrope. Further calculations with graphene and highly oriented pyrolytic graphite (HOPG) substrate have be performed to figure out if structurally separated and electronically decoupled layers are present at the substrate interface. Concerning the electronic properties, we present the calculated bandstructures and density of states and comparisons with the measured differential conductance, which are in good agreement.

DS 20.9 Wed 16:00 P3

Twisted bilayer antimonene — •Stefan Wolff, Roland Gillen, and Janina Maultzsch — Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Antimony has proven to be a promising candidate for two-dimensional (2D) mono-elemental materials. In bulk form, it is a layered crystal comprising sheets of antimony atoms arranged in a hexagonal buckled honeycomb lattice called antimonene. The natural stacking order follows an ABC-pattern, in which each subsequent layer is shifted by one third. Other than many other 2D materials, the interlayer bonds in few-layer antimonene show partially covalent character. Due to this covalent character, changes of the local stacking order via rotation and translation may lead to new interesting features and properties of the material. Density functional theory (DFT) is used to simulate twisted bilayer antimonene structures with different rotation angels and to investigate their physical properties. Moiré patterns and local stacking orders can be found, which lead to a non-uniform bond length distribution. Additionally, our investigation of the charge density shows how the overlap of atomic orbitals in certain areas changes, depending on the proximity of atoms from neighboring layers. A comprehensive understanding of how the properties of twisted bilayer antimonene are modified compared to naturally stacked bilayer antimonene may lead to future applications making use of well-constructed, favorable stacking orders in layered materials.

DS 20.10 Wed 16:00 P3

Determination of circularly polarized light-triggered chiral excitons in organic light harvesting devices — •Otgonbayar Erdene-Ochir, Dirk Hertel, and Klaus Meerholz — Chemistry Department, University of Cologne, Cologne, Germany

Organic-chiroptics have not been a focus of the research area due to the trace amount of circular dichroism (CD) nature has provided in most chiral molecules. However, aggregation of chiral prolinol functionalized squaraine offers giant intrinsic CD behavior. The CD effect is related not only to the difference of left- and right-handed circularly polarized (CP) light absorption for the organic chiral molecule, but also associated with their excitonic nature based on the formation of molecular aggregates. This work discusses the determination of the selective chiral excitons via direct right- and left-handed CP laser radiation. The enantiomer of squaraine derivative (S,S)-ProSQ-C16 is a strongly CD-active material featuring maximum absorbance at ca. 780 nm after thermal annealing of a thin film. We introduced (S,S)-ProSQ-C16 as a p-type active material in a planar heterojunction (PHJ) and bulk heterojunction (BHJ) blend for the photovoltaic devices, together with the fullerenes C60 and PCBM as acceptors, respectively. We used normal-incident transmission Mueller Matrix method to determine the intrinsic CD effects of the thin film. An electronic characterization of the chiral exciton within the PHJ and BHJ systems are quantified. The efficiency of the chiroptical response is estimated by the dissymmetry factor. A systematic correlation between optical and electronic dissymmetry factors will be discussed.

DS 20.11 Wed 16:00 P3

Molecular dynamics simulations of carbon nanomembranes (CNMs): Formation and mechanical properties — •Levin Mihlan, Julian Ehrens, and Jürgen Schnack — Universität Bielefeld, Universitätsstrasse 25, D-33615 Bielefeld

CNMs are made by electron-induced crosslinking of aromatic self-assembled monolayers (SAMs) [1,2]. Their supposedly irregular internal structure cannot be adequately investigated by standard spectroscopic techniques, however, a determination of, e.g. Young's moduli is possible. In order to propose possible internal structures obtained from various initial configurations of the SAM and irradiation processes, we investigate the monolayers with respect to the Young's modulus in terms of classical molecular dynamics calculations using LAMMPS and compare to experimental values. We present three distinct methods to calculate the Young's modulus: Global scaling of all coordinates, stress-strain response from clamped straining and barostatted dynamics. Discrepancies among the methods with regard to vastly different outcomes will be discussed considering finite size effects. CNMs can be used for water filtration, a property that is closely related to the distribution of holes in the membrane [3]. With a hole-detection algorithm for our simulated CNMs we can investigate the hole distributions too and use this as a second observable for comparison with experimental data.

[1] Dementyev, Petr, et al. ChemPhysChem 21.10 1006, 2020
[2] Ehrens, Julian, et al. Phys. Rev. B 103 115416, 2021
[3] Y. Yang, et al. ACS Nano vol. 12 no. 12 pp. 4695-4701, 2018

DS 20.12 Wed 16:00 P3

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

X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS) are two widely used methods to investigate the structure of solid states. Unfortunately, for both techniques, mostly heuristic models are available [1,2,3].

In this contribution, we present the first self-consistent Maxwell-Bloch approach based on Heisenberg equation of motion formalism for the unified description of XANES and EXAFS for 2D solid-state materials and apply it to the exemplary material graphene. For XANES we reproduce the experimentally observed absorption peaks and polarization-dependent selection rules of the included orbitals. Furthermore, the rigorous treatment of the Bloch theorem allows us to calculate the Fourier transformed EXAFS spectrum [2] predicting so far uninterpreted features which have not been assigned within scattering theory [1].

[1] Sayers, Dale E., et al., PRL 27 (1971): 1204
[2] Buades, Bárbara, et al., Optica 5 (2018): 502
[3] Chowdhury, M. T., R. Saito, and M. S. Dresselhaus, PRB 85 (2012): 115410.

DS 20.13 Wed 16:00 P3

Confinement induced coherent phonon softening in Sb2Te3 thin films — •Jonathan Frank[1], Julian Mertens[1], Felix Hoff[1], Mohit Raghuwanshi[2], and Matthias Wuttig[1] — [1]1. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Femtosecond reflection-type optical pump-probe experiments on a thickness-series of MBE-grown Sb2Te3 thin films were carried out to study confinement effects of coherent optical phonons. Therefore, an isotropic detection scheme was applied to investigate the ultrafast dynamics of the LO-phonon mode of A1g-symmetry in Sb2Te3 thin films ranging from 1.3 to 55 nm. The ultrafast response of each thin film contains a distinct coherent feature uncovered by damped harmonic oscillations in the transient reflectivity traces. It is shown that coherent optical phonons are efficiently photoexcited in thin films of only a few quintuple layers. This finding supports the hypothesis that electron-phonon coupling in ultrathin sesqui-chalcogenide films does not fundamentally differ from bulk which is essential for the performance in strongly scaled applications as for example in topological insulators. Furthermore, a slight decrease in phonon-frequency accompanied by a more pronounced decrease in phonon-lifetime is observed in films smaller than ten nanometers; both quantities nearly monotonously decrease with film thickness. We ascribe this phonon softening to a decreased interlayer coupling in films of a few quintuple layers compared to a more bulk-like behavior observed in the thicker films.

DS 20.14 Wed 16:00 P3

Characterization of layer systems by combination of X-ray reflectivity and hyperspectral imaging — •Steffen Bieder[1], Florian Gruber[2], Patrick Schlenz[3], Phillipp Wollmann[2], Christian Albers[1], Susanne Dogan[1], Michael Paulus[1], Nicola Thiering[1], Christian Sternemann[1], and Steffen Cornelius[3] — [1]TU Dortmund, 44227 Dortmund, Germany — [2]Fraunhofer IWS, Winterbergstrasse 28, 01277 Dresden, Germany — [3]Fraunhofer FEP, Winterbergstrasse 28, 01277 Dresden, Germany

Different thin film multilayers consisting of indium tin oxide, zinc tin oxide and silver deposited on flexible PET foils were studied using X-ray reflectivity and hyperspectral imaging aiming for an online quality control of the coatings' manufacturing process. The X-ray reflectivity data measured at beamline BL9 of the DELTA synchrotron radiation source provide detailed information on layer thickness with Angström resolution, roughness and electron density. These results are used to establish statistical models in order to analyze and interpret the data obtained from hyperspectral imaging. Latter is foreseen to be implemented into the foils' production line for in-situ detection of thickness changes during the production process.

The authors acknowledge funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862055. We thank DELTA for providing synchrotron radiation.

DS 20.15 Wed 16:00 P3

Surface second harmonic generation in dielectric nanofilms — •Fatemeh alsadat Abtahi[1], Pallabi Paul[1,2], Sebastian Beer[1], Adriana Szeghalimi[1,2], Stefan Nolte[1,2], and Falk Eilenberger[1,2,3] — [1]Institute of Applied Physics, Friedrich-Schiller-University, Jena, Germany — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany — [3]Max Planck School of Photonics, Jena, Germany

Second-harmonic generation (SHG) is a second-order nonlinear optical process that is not allowed in media with inversion symmetry. However, due to the broken symmetry at the surface, surface SHG can still occur in such materials. We experimentally investigate the surface SHG in the periodic stacks of ultrathin dielectric layers. Uniform, dense and optically homogeneous multilayer stacks of SiO2/TiO2 were grown by Plasma Enhanced Atomic Layer Deposition (PEALD) on fused silica substrates. With this technique individual layers of a thickness of less than 2 nm can be fabricated, increasing the number of SHG-active surfaces substantially. Because of the material discontinuity, in each surface of this structure, the symmetry is broken and surface SHG will occur. By changing the Angle of Incidence (AOI) and having constructive interference between all fundamental/SHG signals from different surfaces, we are able to enhance the surface SHG. We experimentally show that under large angles of incidence > 20 degrees there is substantial SHG, well beyond the level, which can be expected for simple surfaces.

DS 20.16 Wed 16:00 P3

Surface-Enhanced Raman Spectroscopy and Transient Reflectivity of Strained LSMO Thin Films — •Leonard Schüler, Tim Titze, Stefan Mathias, Daniel Steil, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen

The effect of lattice strain on the structural and electronic surface reconstruction of epitaxial $La_{0.7}Sr_{0.3}MnO_3/LaAlO_3$ (LSMO/LAO) thin films has been studied by surface-enhanced optical measurements. Surface sensitivity is achieved by deposition of gold nanoparticles, in which the localized surface plasmon resonance enhances laser electric fields at the surface, enabling surface-enhanced Raman spectroscopy (SERS) and pump-probe reflectivity (SE-PPR) studies of the LSMO films. For this system, SERS reveals a structural surface reconstruction and signals an insulating surface state characterized by strong Jahn-Teller modes which are not present in the conventional Raman spectra of the ferromagnetic metallic LSMO/LAO films. Furthermore, a structural transition of the insulating surface is shown at T*=200-220 K possibly related to charge ordering (CO). SE-PPR indicates that it is possible to photoinduce a ferromagnetic metallic phase at the surface above the assumed CO transition temperature.

DS 20.17 Wed 16:00 P3

In-situ spectroscopic ellipsometry analysis of SiO2 on Si under different atmosphere and temperature — •Xinyu Zhou, Younes Slimi, Stefan Krischok, and Rüdiger Schmidt-Grund — Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Strafte 32, 98693 Ilmenau, Germany

In-situ Spectroscopic ellipsometry has been applied to obtain optical constants and thin film thicknesses of SiO2 on Si under different at-

mospheres (nitrogen, dry air) and temperatures. We found changes in refractive index and thickness of the SiO2 layer under different conditions due to oxidation and material ablation. We further present our recent developments in building up an in-situ ellipsometry system for photo-electrochemical applications.

DS 20.18 Wed 16:00 P3

Spectroscopic Ellipsometry of transition metal oxide thin films — •Nahid Ahmadian[1,2], Teresa I. Madeira[1,2], and Dietrich R.T. Zahn[1,2] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), D-09107, Chemnitz, Germany

Transition metal oxides such as HfO_2 or TiO_2 with bandgaps of 5.3-5.9 eV and 3.0-3.4 eV, are transparent in the visible range of the spectrum, i.e. their extinction coefficient in this range is very low close to zero while the refractive index varies as a function of photon energy. In this work, we tested four dispersion models: Sellmeier, Cauchy, extended Cauchy, and Tauc-Lorentz aiming at understanding the mathematical and physical differences of these approximations, their robustness and limitations in addressing amorphous and crystalline phases of thin films of HfO_2 deposited by atomic layer deposition (ALD) on Si(100) and TiO_2 thin films prepared on Si(100) by magnetron sputtering and spin coating. The spectroscopic ellipsometry measurements were performed using a M-2000 T-Solar from J.A. Woollam. Spectra covering a range of energies 0.7 (IR) − 5 eV (UV) were taken in air at room temperature and analyzed using CompleteEASE. We conclude that multiple oscillators are required to treat the crystalline phases in comparison to the amorphous, and when very good solutions are obtained from all oscillators, the choice to use one or the other is based on complexity: the less the fit parameters the best.

DS 20.19 Wed 16:00 P3

Reaction of Tetrapyrrole Thin Films with Alkali Metals — •Leonard Neuhaus[1], Stefan Renato Kachel[1], Peter Schweyen[2], Mark Hutter[1], Maik Schöniger[1], Florian Münster[1], Lukas Ruppenthal[1], Jan Herritsch[1], Marie-Irene Albus[1], Martin Bröring[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Anorganische und Analystische Chemie, Technische Universität Braunschweig, Germany

Tetrapyrroles such as porphyrins play an import role in living organism and for various modern technologies. While most previous publications related to tetrapyrrole thin films focus on transition metal complexes, we want to expand the field by exploring the reaction of various tetrapyrrole films with alkali metals. For this purpose, we prepared multilayer films of tetraphenylporphyrin and an octaalkylcorrol on a Au(111) surface and studied their reactions with Li and Cs, thus covering the extremes of the lightest and heaviest stable alkali metal. For all studied systems, X-ray photoelectron spectroscopy (XPS) showed, changes in the N 1s region that indicate formation of the corresponding tetrapyrrole metal complexes. Complementary studies with temperature programmed reaction (TPR) provided unambiguous mass spectrometric evidence for the formation of the metal complexes. TPR also showed that the number of alkali metal atoms attached to a tetrapyrrole ligand can exceed the number of pyrrolic hydrogen atoms in the free-base tetrapyrrole.

DS 20.20 Wed 16:00 P3

Thermoelectric Characterization of Polymer Thin Films with Ag-nanowire Additives — •Sohraab Scherzad[1], Marie Siegert[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Along the process of power conversion from primary energy carriers vast amounts of waste heat in the low and mid temperature range occur. A possible solution to recover this waste heat is offered by thermoelectric generators which rely on the Seebeck effect and are able to directly convert thermal into electrical energy. Polymeric semiconductors, operating in this temperature regime, offer a sustainable and low-cost alternative to inorganic thermoelectrics. Their characteristics include a sufficiently low thermal conductivity κ, but also a low electrical conductivity σ, due to the low charge carrier concentration and generic disorder. Here we report on composite thin films made of Ag-nanowires embedded in PEDOT:PSS polymer matrices, which lead to changes in the electrical conductivity compared to pure PEDOT:PSS. Ag-nanowires are considered to be a suitable additive for increasing σ of the resulting composite and its impact on κ will also be studied. First results on the thermoelectric properties of this material combination will be presented together with structural information obtained by X-ray diffraction and atomic force microscopy. Based on this complementary information we will critically discuss the potential of the presented approach for application in TEGs.

DS 20.21 Wed 16:00 P3

Plasmonic-induced Thermoelectric Effects in Metal-organic Hybridstructures — •Lucca Macher[1], Paul Hoppstock[1], Maximilian Frank[1], Maximilian Rödel[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Local heat generation by plasmonic excitations in noble metal nanoparticles is of high technological interest for numerous applications such as photo-thermal chemistry or cancer therapy. In this work we utilize this approach to create a thermal gradient by the absorption of light in metal-organic hybrid structures. The latter are based on arrays of nanostructured gold and silver triangles in combination with solution processed p-type PEDOT:PSS films. As we can demonstrate, a defined temperature enhancement and thus, gradient evolves upon resonantly exciting local plasmons in the Au or Ag nanoparticle arrays. The amplitude of this enhancement amounts to $\Delta T = 0.5$ K for an incident light power of 1.4 mW/mm^2. Accordingly, this plasmon-induced temperature gradient which is aligned along the PEDOT:PSS polymer layers results in a significant enhancement of the thermovoltage to $V_T = 24\ \mu$V/K as compared to neat PEDOT:PSS ($V_T = 12\ \mu$V/K). An application-oriented approach was carried out as well, using arrays of nanostructured gold triangles covered by a transparent polymer-gel electrolyte PEGMA/BEMA in a window-like device architecture. A temperature gradient of $\Delta T = 0.1$ K for an incident light power of 1.8 mW/mm^2 was determined along the PEGMA/BEMA layer.

DS 20.22 Wed 16:00 P3

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

Spin-crossover (SCO) complexes are regarded as promising materials in applications such as spintronics, molecular electronics and ultra-high-density memory systems. They can be switched by external stimuli, e.g., change of temperature, pressure, or illumination with light. In the investigated complexes switching occurs between diamagnetic low-spin (LS) and paramagnetic high-spin (HS) species by either a simple SCO, or a valence tautomeric (VT) transition accompanied by a SCO. While the mentioned applications seem promising, one big challenge that needs to be overcome is the transfer of the systems from solution or bulk towards thin films or even monolayers on well-defined surfaces. Six-coordinate iron(II) complexes have been used as SCO materials, whereas six-coordinate Co complexes with redox active dioxolene ligands were chosen as VT materials. Both materials can be attached to the surface via a bidental phenanthroline ligand containing moieties suitable for bonding to the substrate. Here we report a step by step formation of single-layer films on Au(111) surfaces. The thus created specimens were characterized by atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and near edge x-ray absorption fine structure (NEXAFS).

DS 20.23 Wed 16:00 P3

Chern number control in quantum anomalous Hall insulators by external fields — •Yuriko Baba[1,2], Francisco Domínguez-Adame[1], and Rafael A. Molina-Ferández[2] — [1]GISC, Departamento de Física de Materiales, Universidad Complutense, E–28040 Madrid, Spain — [2]Instituto de Estructura de la Materia, IEM-CSIC, E–28006 Madrid, Spain

Topological magnetic insulators have been discovered as a new platform for observing Quantum Anomalous Hall states with high Chern number C. In three-dimensional structures of stacking layers of magnetically doped and undoped topological insulators of Bi2(Se,Te)3, the number of chiral edge channels can be controlled by the width and number of layers and by the doping concentration. This has been recently measured by Zhao et al. [1] in Cr doped samples, showing this feature up to C = 5.

In this theoretical work, we explore the possibilities of tuning the chiral channels of the aforementioned materials in the presence of electric fields in multilayered structures. The external field tunes the Chern

number and changes the number of topological channels dynamically without the need of replacing the sample to modify the Chern number. The tuneability has a remarkable impact on the transport properties of pristine and disordered samples.

[1] Zhao, Y. F. et al., Nature, 588 (2020) 419

DS 20.24 Wed 16:00 P3

topological magnons and thermal hall conductivity in 2D magnets — •Hamid Nouri and Hongbin Zhang — Technical University of Darmstadt, 64287 Darmstadt, Germany

Two-dimensional (2D) materials provide a fascinating playground for emergent phenomena driven by enhanced thermal and quantum fluctuations, in particular the nontrivial topological phases with the associated dissipationless transport properties. For 2D magnetic insulators, magnons can also host Dirac and Weyl points with nonzero Berry curvature, leading to finite thermal Hall conductivities. In this work, based on the linear response spin-wave theory, we investigated a Hamiltonian formulated on 2D lattices comprising the Heisenberg exchange, Dzyaloshinskii-Moriya interaction (DMI) interactions, single-ion anisotropy, external magnetic fields, and found that the gapped magnon bands exhibit nonzero Chern numbers of *1 due to finite DMI which acts like effective spin-orbit coupling. The thermal Hall conductivity is evaluated based on the Boltzmann transport theory, suggesting a novel approach to designing 2D thermal management materials. The realization of such Hamiltonians in experimentally available 2D materials will be discussed as well.

DS 20.25 Wed 16:00 P3

Bottom-up preparation of large area van-der-Waals heterostructures by the subsequent growth of 2D transition metal dichalcogenides layers — •Devendra Pareek[1], Marco A. Gonzalez[1], Nedal Grewo[1], Marten L. Janssen[1], Leon A. Gräper[1], Kumarahgiri Arunakiri[1], Kayode. L. Alimi[1], Martin Silies[1,2], Jürgen Parisi[1], Levent Gütay[1], and Sascha Schäfer[1] — [1]Ultrafast Nanoscale Dynamics, Institute of Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [2]Institute for Lasers and Optics, University of Applied Sciences Emden/Leer, Emden, Germany

We report the preparation of as-grown two-dimensional transition metal dichalcogenides (2D-TMDC) heterostructures from a processing route employing a combination of atomic layer deposition of monolayer MoS_2 and solution-based processing of ultrathin $Mo(S/Se)_2$ and $W(S/Se)_2$ films. Grown on centimeter-scale sapphire substrates, spatially uniform optoelectronic characteristics of the individual TMDC layers and heterostructures are demonstrated down to micrometer length scales using photoluminescence, Raman spectroscopy, and light-beam-induced current measurements. Preliminary observations on enhanced photogenerated currents in MoS_2-MoS_2/WS_2 lateral heterostructures demonstrate the suitability of this approach for the preparation of functional devices on macroscopic length scales. Finally, we also discuss the possibilities to synthesize these compounds at temperatures below 400 °C, making them suitable for a broad range of substrate materials.

DS 20.26 Wed 16:00 P3

Twist-angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide and graphene/topological insulator heterostructures — •Thomas Naimer[1], Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Uni Regensburg, Regensburg, Germany — [2]Pavol Jozef Šafárik University, Košice, Slovakia

We investigate the proximity-induced spin-orbit coupling in twisted heterostructures of graphene/transition-metal dichalcogenides (MoS_2, WS_2, $MoSe_2$, and WSe_2) as well as graphene/topological insulators (Bi_2Se_3 and Bi_2Te_3) from first principles. To correct for strain induced band offsets, we apply a perpendicular electric field. The resulting corrected band structure is then fitted around the Dirac point to an established spin-orbit Hamiltonian, yielding the twist angle dependencies of the (Rashba and valley-Zeeman) spin-orbit coupling. This work was funded by the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), 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 20.27 Wed 16:00 P3

Valley depolarization of excitons in encapsulated $MoSe_2$-WSe_2 heterostructures with controlled moiré potentials — •Andreas Beer[1], Anna Weindl[1], Niclas Maier[1], Antony George[2], Andrey Turchanin[2], and Christian Schüller[1] — [1]Universität Regensburg — [2]Friedrich-Schiller-Universität Jena

Our focus is the investigation of the temporal and spatial dynamics of interlayer excitons in $MoSe_2$-WSe_2 heterostructures with well-defined moiré potentials, based on CVD grown samples. The so called hot pickup method enables us to fabricate such heterostructures out of CVD grown triangulars in a controlled, dry, PDMS-free and easy way.

To understand the valley depolarization mechanism in TMDC monolayers and heterostructures we perform time resolved pump probe measurement. First measurements on twisted TMDC exfoliated heterostructures reveal twist-angle-dependent decay times of the interlayer exciton.

DS 20.28 Wed 16:00 P3

Protection of QSHI indenene from air via intercalation — •Cedric Schmitt[1,2], Jonas Erhardt[1,2], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

In the search for new quantum materials, ultrathin metals are interesting as they push bulk properties to the 2D limit and foster novel quantum effects. Unfortunately, these systems are prone to oxidation in air, making them useless for quantum transport devices. Metal intercalation is a relatively new capping method, that utilizes graphene, an inert quantum material that can be easily produced by heating of a SiC substrate [1,2]. Hereby, the metal is intercalated between the SiC/graphene layer, thus forming freestanding graphene, which is believed to protect the intercalated layers against oxidation [3]. Hitherto studies focused mainly on identifying stable allotropes but lacking a detailed investigation of metal coverage and oxidation [3]. Here, we study the intercalation of indenene, a recently discovered QSHI on a triangular lattice [4]. First experiments indicate the indium layer to remain intact upon air exposure, indeed pointing to an effective protective function of the overlayer graphene.

[1] K. S. Novoselov et. al. Science 306, 666 (2004)
[2] C. Berger et. al. J. Phys. Chem. B 108, 19912 (2004)
[3] N. Briggs et al. Nat. Mater. 19, 637-643 (2020)
[4] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)

DS 20.29 Wed 16:00 P3

Electronic Structure of $[(SnSe)_{1+\delta}]_m(TiSe_2)_n$ investigated by Photoelectron Spectroscopy — •Niels Rösch[1], Fabian Göhler[1], Danielle M. Hamann[2], David C. Johnson[2], and Thomas Seyller[1] — [1]Technische Universität Chemnitz, Institut für Physik, 09126 Chemnitz — [2]University of Oregon, Department of Chemistry, Eugene OR 97401

The Modulated Elemental Reactants (MER) synthesis is a new method for producing multilayer heterostructures. A precursor is created in MER by using consecutive physical vapour deposition. The precursor's structure and composition can be deliberately changed to mimic the desired heterostructure. After that, the precursor is crystallized by annealing it at low temperatures in an inert environment. Low temperatures allow thermodynamically metastable films to form, albeit at the cost of turbostratic rotational disorder between layers. By systematically modifying the stacking sequence of individual layers, this approach can be used to create a succession of layered heterostructures.

X-ray photoelectron spectroscopy was used to investigate the electrical structure of a sequence of $[(SnSe)_{1+\delta}]_m(TiSe_2)_n$ heterostructures [1]. It is demonstrated that electrons are transferred from the SnSe layers to the $TiSe_2$ layers. Understanding charge transfer in heterostructures is important for future applications, as controlled stacking of the heterostructure may allow for targeted doping.

[1] Göhler, F., Hamann, D. M., Rösch, N., et al., J. Mater. Res. 34 (12): (2019)

DS 20.30 Wed 16:00 P3

Atomistic Simulations of Defects Production Under Ion Irradiation in Epitaxial Graphene on SiC — •Mitisha Jain[1], Silvan Kretschmer[1], Katja Höflich[2,3], Joao Marcelo J. Lopes[4], and Arkady Krasheninnikov[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Ferdinand-Braun Institut gGmbH, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und

Energie GmbH, Berlin, Germany — [4]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

In this work, using atomistic simulations at the analytical potential and density-functional theory (DFT) levels, we theoretically study defect production in EG on SiC by ion beams (He and Ne ions). We explicitly consider the effects of the substrate (bulk SiC) on the response of graphene to irradiation. Since the substrate affects the number of displaced carbon atoms and vacancy types in EG, we present information about the number, types and location of defects produced in each layer of EG to guide the experiment in tailoring the defect production. Motivated by the He FIB experiments (aiming at nucleation sites of h-BN growth, operating at 30 keV), our considerations apply to the typical ion energies used in HIM, that is 10-30 keV.

DS 20.31 Wed 16:00 P3

Low energy ion induced effects on core-shell nano particles — •Julian Lisson, Shiva Choupanian, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Ion irradiation can be used for manipulating the shape and properties of nanomaterials. However, the comportment of nano materials irradiated with energetic ions differs from bulk and thin films due to the mesoscopic properties of nanoparticles. The succeeding effects such as sputtering and ion beam mixing are strongly coupled and are dependent on the properties of the irradiated target. In this study, the effect of Ga+ ions with an energy range of 10-30 keV on different nanomaterials of Au, Ag, Au-Ag mix, and core-shell nanoparticles dispersed on Si substrates has been investigated. The sputter yield for each nanomaterial has been measured. Comparing the sputter yield and morphology changes of the nanoparticles, we observe that the ion beam mixing at the interface of the Au-Ag core-shell nano particles is prominent. The sputter yield dependence is changing when ion beam mixing is occurring and leads to dissimilar morphology changes of the core-shell nanoparticles due to preferential sputtering.

DS 20.32 Wed 16:00 P3

Lattice dynamics in tuneable thin films with Ruddlesden-Popper structure — •Veronica Goian[1], Natalie Dawley[2], Jingshu Zhang[2], Christelle Kadlec[1], Nathan D. Orloff[3], Reinhard Uecker[4], Steffen Ganschow[4], Darrell G. Schlom[2,5], and Stanislav Kamba[1] — [1]Institute of Physics ASCR, Prague, Czech Republic — [2]Department of Materials Science and Engineering, Cornell University, Ithaca, NY, USA — [3]National Institute of Standards and Technology, Boulder, CO, USA — [4]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [5]Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY, USA

In this work, we will compare the phonon dynamics of $(SrTiO_3)_6SrO$ (SrRP6) thin film with $(SrTiO_3)_5(BaTiO_3)_1SrO$ (BaRP6) and $Sr_{5/6}Ba_{1/6}TiO_3$ (SBT) thin films, all deposited on (110)$DyScO_3$ substrates. The XRD measurements and the rocking curves prove the thin films are single phase and epitaxially grown on the substrates. The lattice dynamics of the thin films were determined using THz and IR spectroscopies down to 10 K. Many phonons exhibit anomalies near temperatures of the ferroelectric phase transitions. We found out that the 100 nm BaRP6 and SBT thin films have T_C about 40-50 K higher than previously studied 50 nm thin films, which is due to slightly relaxed strain in the thin films. We will also compare the temperature behavior of the complex permittivity of BaRP6 and SBT thin films with behavior of $Ba_xSr_{1-x}TiO_3$ (x=0.1..0.6) ceramics and will discuss the reason for high tuneability of permittivity and low dielectric loss in strained thin films.

DS 20.33 Wed 16:00 P3

Stabilized ferromagnetism in LPCMO thin films by using buffer layers — •Pia Henning[1], Karen Stroh[1], Vitaly Bruchmann-Bamberg[1], Oleg Shapoval[2], and Vasily Moshnyaga[1] — [1]Erstes Physikalisches Institut, Georg-August-Universitat-Göttingen, Gottingen, Germany — [2]IIEN, Academy of Sciences of Republic Moldova, Chisinau, Republic of Moldova

$(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3$ (LPCMO) is an A-site substituted perovskite manganite and is mostly known for the colossal magnetoresistance (CMR) effect. Relatively thick LPCMO films ($d \approx 50-100$ nm) with a coupled ferro-to-paramagnet and a metal-to-insulator transition (MIT) and CMR can be heteroepitaxially grown on MgO(200) substrates, where a relaxed growth due to misfit dislocations is achieved. However, very thin LPCMO films with $d \lesssim 20$ nm on MgO(200) do not show a MIT and CMR. On the alternative substrate $SrTiO_3$ (100), LPCMO grows coherently strained and with good surface morphology, but lacks an MIT and CMR even for $d \lesssim 50$ nm.
To enable high-quality LPCMO thin film growth on $SrTiO_3$ substrates, the introduction of a buffer layer to bridge the lattice mismatch of film and substrate is inevitable. Based on this, we investigate the growth of $LaAlO_3$ (LAO) buffer layers on $SrTiO_3$ and the influence of LAO buffer layers on the growth of LPCMO in order to improve the magnetic and electric properties. Specifically, the interplay of buffer and film thickness is studied. It is demonstrated the possibility of high quality thin film growth of LPCMO on buffered STO and a stabilization of the ferromagnetic-metallic phase.

DS 20.34 Wed 16:00 P3

Electronic Reconstruction and Anomalous Hall Effect at the $LaAlO_3/SrRuO_3$ Interface — •Merit Spring[1], Ji Soo Lim[1], Martin Kamp[1], Louis Veyrat[2], Pavel Potapov[2], Axel Lubk[2], Bernd Büchner[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany — [2]Leibniz Institute for Solid State and Materials Research and Würzburg-Dresden Cluster of Excellence ct.qmat, 01069 Dresden, Germany

4d and 5d transition metal oxides are a promising class of materials for topological phases in the context of electron correlations. Recently, the ferromagnetic metal $SrRuO_3$ (SRO) grown on a $SrTiO_3$ (STO) (001) substrate has been reported to exhibit electronic-reconstruction induced interfacial charge pinning accompanied by a topological transition of its electronic bands when capped with a $LaAlO_3$ (LAO) layer [1]. LAO is a polar oxide and the electronic reconstruction in a heterosystem of LAO/STO caused by the polar discontinuity at the interface is well known. For the LAO/SRO system a similar behaviour is expected and charge is thought to be accumulated at the very interface giving rise to strong inversion-symmetry breaking and hence change in the momentum-space topology [1]. Here we show the observation of signatures of an anomalous Hall effect in 4uc SRO films capped with LAO but also with non-polar STO. We correlate these findings with angle-dependent XPS data that allow for depth-profiling the oxidation state of ruthenium in both systems.
[1] Thiel, T. C. et al., Phys. Rev. Lett. 127, 127202 (2021)

DS 20.35 Wed 16:00 P3

Epitaxial growth of IrO2(110) thin films on TiO2(110) substrates by pulsed-laser-deposition — •Tim Waldsauer[1], Philipp Kessler[1], Theodore Pellegrin[1], Christopher Reiser[1], Ralph Claessen[1], Vedran Jovic[2], and Simon Moser[1] — [1]JMU Physikalisches Institut, am Hubland, Würzburg, Germany — [2]GNS National Isotope Center, Gracefield Rdd, Gracefield, New Zealand

Iridium dioxide (IrO2), a state-of-the-art catalyst for the electrocatalytic oxygen evolution reaction in water splitting, has recently been shown to exhibit exotic physical phenomena such as the inverse spin Hall effect. The latter is supposed to promote easy switching of its majority charge carriers. For both fundamental spectroscopic studies as well as device applications, IrO2 samples of high bulk and surface crystalline order are required. Here, we present a growth study of rutile IrO2(110) thin films on TiO2(110) substrates by pulsed-laser-deposition (PLD). Film characterization by AFM, RHEED and XPS shows stochiometric growth of thin films with high bulk crystallinity but a granular surface at higher thicknesses. Strategies to enhance the surface quality, e.g., through utilization of an oxygen plasma are outlined and first results are presented.

DS 20.36 Wed 16:00 P3

2D electronic states at Fe_xO_y/STO interfaces — •Pia M. Düring[1], Paul Rosenberger[1,2], Lutz Baumgarten[3], Fatima Alarab[4], Frank Lechermann[5], Vladimir N. Strocov[4], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Fakultät Physik, Technische Universität Dortmund, 44221 Dortmund, Germany — [3]FZ Jülich GmbH, PGI-6, 52425 Jülich, Germany — [4]PSI, Swiss Light Source, CH-5232 Villingen PSI, Switzerland — [5]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

Oxide interfaces play an important role in investigating phenomena like 2D electronic states which can feature properties like magnetism, superconductivity or the spin Hall effect. While 2DEGs have been reported for various oxide systems like LAO/STO or EuO/STO, the direct experimental evidence for the counterpart, the 2DHG, is still

lacking. Using our UHV-MBE system, we grow high-quality oxide heterostructures to investigate these properties using synchrotron radiation. Here presented are the results of resonant photoelectron spectroscopy measurements that reveal the emergence of different 2DESs at Fe_xO_y/STO interfaces which suggests a dependence of the 2D interface properties on the oxidation state of Fe.

DS 20.37 Wed 16:00 P3

Stabilization of ferromagnetic metallic ground state in epitaxial $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ /$SrTiO_3$ thin films by using buffer layers — •Pia Henning[1], Karen Stroh[1], Vitaly Bruchmann-Bamberg[1], Oleg Shapoval[2], and Vasily Moshnyaga[1] — [1]Erstes Physikalisches Institut, Georg-August-Universitat-Göttingen, Gottingen, Germany — [2]IIEN, Academy of Sciences of Republic Moldova, Chisinau, Republic of Moldova

$(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ (LPCMO) is an A-site substituted perovskite manganite, mostly known for the colossal magnetoresistance (CMR) effect. Relatively thick, d=50-100 nm, and stress-free LPCMO films with coupled ferro/paramagnetic and metal/insulator transition (MIT) and CMR $\sim 10^4$% can be heteroepitaxially grown by the metalorganic aerosol deposition technique on MgO(200) substrates, where strain relief occurs due to misfit dislocations. However, thin LPCMO films d<20 nm on MgO(200) do not show MIT and CMR. Alternatively, LPCMO/SrTiO3 (LPCMO/STO) films grow coherently strained and with smooth surface morphology, however lacking the MIT and CMR even for d>50 nm. To obtain epitaxial LPCMO films with optimal metal-insulator transition sharpness and temperature we have employed a strain-engineered $LaAlO_3$ buffer layer to bridge the lattice mismatch of the LPCMO film and $SrTiO_3$(100) substrate. The influence of $LaAlO_3$ buffers on the magnetic and electric properties of epitaxial LPCMO films was studied. A high-quality growth of LPCMO/LAO/STO films and stabilization of the ferromagnetic-metallic phase for 10 nm thick LPCMO films were demonstrated.

DS 20.38 Wed 16:00 P3

Metal-insulator transition in $AgSb_{1-x}Sn_xTe_2$ alloys — •Christian Teichrib and Matthias Wuttig — I. Physikalisches Institut (IA)

Metal-insulator transitions describe the localisation of charge carriers upon the change of a physical parameter. They can occur as a result of electron correlations (Mott transition) or disorder (Anderson transition) but a distinction between these two mechanisms is generally difficult and often both effects play a role in the transition. Phase change materials show a multitude of remarkable properties that make them suitable for the investigation of localisation phenomena. Their density of states at the Fermi level can be varied through chemical composition and disorder can be tuned through thermal annealing. This allows for the electrical resistivity to be modified over several orders of magnitude and a transition from a metallic to an insulating state to occur.
We present electrical transport and structural data for $AgSb_{1-x}Sn_xTe_2$ alloys where a metal-insulator transition is observed upon variation of the stoichiometry. The nature of the transition is investigated using the temperature dependence of the resistivity, magnetoresistance data, and the Hall effect.

DS 20.39 Wed 16:00 P3

Cryogenic Transport And Dielectric Properties Of Atomically Thin 2D-Polar Metals — •Sven Bökemeier[1], Pierre-Maurice Piel[1], Jakob Henz[1], Margaux Lassunière[1], Joshua Robinson[2], Siavash Rajabpour[2], Alexander Vera[2] und Ursula Wurstbauer[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

2D layered materials are of great interest due to their electronic and optical properties that can be manipulated to a high degree. A novel class of atomically thin materials are 2D polar metals such as 2D Ga or 2D In and their ternary alloys that exhibit fascinating properties like strong nonlinear optical properties emerging by giant second harmonic generation [1], epsilon near zero behavior in the visible and NIR range [2] and alloy dependent superconductivity [3]. Intriguingly, 2D Ga exhibits a superconducting phase transition around 4K, while 2D In remains a metal down to < 800mK [3]. The 2D polar metals are prepared via confinement hetero-epitaxy (CHet) by intercalating metals between epitaxial graphene and the hosting SiC crystal resulting in atomically thin half-van der Waals materials [1]. We report on combined temperature dependent transport and spectroscopic ellipsometry experiments in order to a develop a better understanding of the alloy dependent emerging superconductivity of thin 2D Ga and 2D GaIn films. [1] M. A. Steves et al. Nano Lett. 2020, 20, 11, 8312*8318. [2] K. Nisi et al. Adv. Mater. 2021, 2104265 [3] S. Rajabpour et al. Adv. Funct. Mater. 2020, 2005977

DS 20.40 Wed 16:00 P3

Magnetic Field-Dependent Thermal Conductivity in Manganite Thin Films — •Vitaly Bruchmann-Bamberg, Karen Stroh, Pia Henning, and Vasily Moshnyaga — I. Physik. Inst. Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

In perovskite manganites strong electron-phonon and spin-phonon coupling give rise to intriguing magneto-electric phenomena like colossal magnetoresistance (CMR), i.e. reduction of electrical resistivity by several orders of magnitude in an applied magnetic field of few Tesla. Since thermal conductivity of a solid contains both lattice and electronic contributions, a question of its manipulation by an external magnetic field can be addressed in CMR manganites.

Here we present temperature- and magnetic-field-dependent measurements of thermal conductivity by means of 3ω-technique in $(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3$/MgO(100) thin films with a CMR ratio of [R(0T)-R(5T)]/R(5T)$\approx 10^4$%. The observed significant change of the thermal conductivity, κ, in magnetic field $[\kappa(5T)- \kappa(0T)]/\kappa(0T) = 16\%$ close to $T_C \approx 200$K is caused by the electronic contribution in agreement with the Wiedemann-Franz law.

DS 20.41 Wed 16:00 P3

Phonon-dominated energy transport in purely metallic thin films — •Marc Herzog[1], Alexander von Reppert[1], Jan-Etienne Pudell[1,2], Carsten Henkel[1], Matthias Kronseder[3], Christian Back[3,4], Alexei Maznev[5], and Matias Bargheer[1,6] — [1]Inst. f. Physik & Astronomie, Universität Potsdam, Germany — [2]European XFEL, Schenfeld, Hamburg, Germany — [3]Inst. f. Experimentelle & Angewandte Physik, Universität Regensburg, Germany — [4]Fakultät f. Physik, Technische Universität München, Germany — [5]Departent of Chemistry, MIT, Cambridge, USA — [6]Helmholtz-Zentrum Berlin, Germany

In various branches of physical sciences it is assumed that electrons are the main carriers of thermal energy in metals. We use ultrafast x-ray diffraction to quantify the energy exchange among the metallic constituents in nanoscale thin films after laser excitation. Modeling the data with two-temperature models describing the energy exchange between non-equilibrium electrons and phonons provides clear evidence that phonons dominate the heat transport within gold films thinner than approx. 10 nm. Our fundamental experimental findings shifts the paradigm of energy being solely transported by electron in noble metals. These results may be relevant for the description of non-equilibrium thermal transport in diverse fields ranging from thermal management in nanoelectronics, spin-caloritronics and ultrafast spin dynamics to photothermal processes and plasmonic chemistry.

DS 20.42 Wed 16:00 P3

Combinatorial Synthesis of $Pb_{1-x}Sn_xSe$ Films with Sputter Deposition — •Thomas Schmidt, Peter Kerres, and Matthias Wuttig — RWTH Aachen University, Aachen, Germany

PbSe and SnSe are two chalcogenides with a wide range of applications of their properties, in particular as thermoelectrics. Interestingly, these two iso-electronic materials employ different bonding mechanisms. While at room temperature SnSe utilizes covalent bonds, PbSe is characterized by a more unconventional bonding mechanism, coined metavalent bonding. Therefore, we expect significant property changes upon crossing the border between those two bonding mechanisms. Such a change opens up the possibility to tailor material properties with sample stoichiometry. We have thus studied optical and electrical properties of $Pb_{1-x}Sn_xSe$ films as a function of stoichiometry. Effective sample-production has been employed to facilitate this analysis. In this study the compositions around x=0.5, at which a structural transition is expected, are confocally sputtered and subsequently analyzed. The two targets PbSe (cubic structure) and SnSe (orthorhombic structure) were focused on the different ends of the 7.5 cm long Si-substrate. The resulting stoichiometry gradient in the sample was determined by energy dispersive X-ray spectroscopy and linked to the evolution of structure (X-ray diffraction) and optical properties (spectroscopic ellipsometry and reflectometry).

DS 20.43 Wed 16:00 P3

Growth of Crystalline High-Entropy Alloy thin Films by

Magnetron Sputtering — •Holger Schwarz[1], Thomas Uhlig[2], Eric Wong[1], Peter Henning[1], Guntram Wagner[2], and Thomas Seyller[1] — [1]Institute of Physics, Faculty of Natural Sciences, TU Chemnitz, 09126 Chemnitz, Germany — [2]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, TU Chemnitz, 09126 Chemnitz, Germany

Multicomponent alloys of at least four elements with near equimolar percentage were first reported and investigated by Cantor et al. in 2004 [1] and are nowadays often referred to as High-Entropy Alloys (HEAs) [2]. This group of materials has raised high attention in the field of material research due to its almost infinite possibilities of element combination and resulting physical properties. We demonstrate the fabrication of crystalline HEA thin films on MgO(100) and Al_2O_3(0001) single crystal substrates from homemade targets via magnetron sputtering. Low electron energy diffraction and X-ray diffraction experiments confirmed the formation of single phase crystalline HEA films. The surface elemental composition is investigated by X-ray photoelectron spectroscopy whereas the bulk stoichiometry is measured by energy dispersive X-ray spectroscopy. Angle resolved photoemission spectroscopy was used to investigate the band structure of the thin films.

[1] B. Cantor, I. Chang, P. Knight, A.Vincent, Mat. Sci. Eng. A, 213-218, 375-377 (2004)
[2] D.B. Miracle, JOM, 2130-2136, 69 (2017)

DS 20.44 Wed 16:00 P3

Different approaches to deposit tungsten-doped vanadium dioxide by ion-beam sputter-deposition — •Jill Kessler, Sebastian Leonard Benz, Isabel Müller, Martin Becker, and Sangam Chatterjee — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

The complexity of the phase diagram of vanadium oxides makes the reproducible growth of thin films of defined phases by nonequilibrium techniques challenging. Here, we discuss thermochromic VO_2, which exhibits a significant change in optical transparency and reflectivity and, thus, is an ideal candidate for the use in smart windows. However, the bulk phase transition temperature of 68 °C is too high for useful applications. Doping VO_2 with tungsten drives the thermochromic key measures close to the desired range.

We present different approaches for tungsten doping of VO_2 based on ion-beam sputter-deposition. We employ tungsten screws that are inserted into the vanadium target. Furthermore, a pre-doped vanadium target is used. In another approach we employ two targets of vanadium and tungsten, respectively, to be sputtered simultaneously. Here, a compositional gradient allows for identification of the optimum doping concentration. The different approaches are compared regarding thin film properties and overall reproducibility of the growth process.

Raman spectroscopy and X-ray photoelectron spectroscopy provide structural and compositional analysis. UV/Vis/NIR spectroscopy yields the thermochromic performance.

DS 20.45 Wed 16:00 P3

Enhanced amorphization of Cu-Sn-I alloy thin films fabricated by reactive magnetron sputtering — •Christiane Dethloff, Sofie Vogt, Tillmann Stralka, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Leipzig, Deutschland

CuI is a promising p-type semiconductor for optoelectronical applications due to various advantageous material properties such as transparency in the visible spectrum [1] and its earth abundant, cheap and non-toxic constituents. Growth of amorphous layers of CuI by solution processing has already been reported [2, 3]. The feasibility of deposition of the amorphous Cu-Sn-I alloy has not yet been demonstrated for a physical, scalable process, such as sputtering.

We present our investigations of the influence of the process parameters during the deposition of a Cu-Sn-I-alloy using reactive co-sputtering of Cu and Sn in a reactive iodine ambient. A dependence of the growth rate, the thin films morphology and the electrical properties on the process parameters i.e. the magnitude of the electrical power applied at the sputtering sources, the iodine partial pressure and the chamber pressure. A decrease of crystallinity was observed by XRD measurements for increasing sputtering power applied on the tin target as well as with increasing chamber pressure. LSM and AFM measurements yielded root-mean-square surface roughnesses below 10 nm.

[1] M. Grundmann *et al.* Phys. Status Solidi A 210, 1671 (2013);
[2] H. Wu *et al.* Appl. Phys. Lett. 118, 222107 (2021);
[3] T. Jun *et al.* Advanced materials 30, e1706573 (2018).

DS 20.46 Wed 16:00 P3

Overcoming the integration issues between 2D materials and waveguides — •Oscar Camacho Ibarra[1], Ioannis Caltzidis[1], Selim Scharmer[2], Samuel Gyger[2], Marc Sartison[1], and Klaus D. Jöns[1] — [1]HQPD lab, Department of Physics, Paderborn University, Germany — [2]Quantum Nanophotonics, KTH Royal Institute of Technology, Sweden

To achieve fully operational quantum photonic integrated circuits, developing a scalable platform capable of supplying an efficient coupling between single-photon emitters and photonic circuitry is essential. A hybrid approach is the most favorable to integrate single-photon emitters with other on-chip components since the advantages of each material platform are exploited. Single-photon emitters hosted in 2D materials are emerging technologies and promising candidates for future scalable photonic circuits. However, the coupling of light from these emitters into waveguides remains challenging: In particular, higher coupling efficiency and reduction of spectral jitter are needed. Both issues can be simultaneously overcome by implementing a cavity in the photonic circuit. In this work, 1D photonic crystal cavities were designed and simulated for later integration of 2D emitters. These photonic crystal cavities are designed to be efficiently coupled to waveguide modes, and they possess high*quality factors and small mode volumes, resulting in prominent Purcell factors. Furthermore, the cavity geometrical structure can act as nucleation sites for strain*driven single-photon emitters, allowing a self-alignment process between emitter and cavity.

DS 20.47 Wed 16:00 P3

Propagation and manipulation of Bloch Surface Waves and Bloch Surface Wave Polaritons in ZnO — •Sebastian Henn, Simon Briesenick, Chris Sturm, and Marius Grundmann — 1Universität Leipzig, Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Linnéstr. 5, 04103 Leipzig, Germany

In this contribution we demonstrate experimentally the control of the propagation of Bloch Surface Waves (BSW) in the transparent spectral range and Bloch Surface Wave Polaritons (BSWP) in the vicinity of excitonic transitions in ZnO. BSWP are bosonic quasi-particles originating from the strong coupling between BSW and excitons and exist along the ambient interface of a distributed Bragg reflector (DBR) with a thin ZnO top layer [1]. Using shallow optical diffraction gratings with sub-micron sized lattice constant, incident light is coupled into and out of the Bloch modes, which propagate along the surface interface between the gratings. Depending on the geometry of the sample and roughness of the surface layer the low-loss nature of evanescent BSW allows long-range lateral propagation of BSWP, on the order of micrometers, making this an interesting candidate for on-chip polaritonic devices. We determine the propagation lengths and test the coupling efficiency of the gratings, which are modelled using RCWA compuations.

[1] S. Henn et al., New J. Phys. 23, 093031 (2021)

DS 20.48 Wed 16:00 P3

Improvement of the Architecture of Water-Based Dye-Sensitized Solar Cells — •Sara Domenici, Andreas Ringleb, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Dye-sensitized solar cells (DSSCs) have emerged as a possible alternative technology for the conversion of sunlight into electrical energy. Aqueous electrolytes would considerably increase their sustainability. Aside from chemical instabilities, the power conversion efficiencies of aqueous DSSCs remain significantly lower compared to other DSSCs. One main problem which is dealt with in the present work, consist in low diffusion coefficients of appropriate redox couples. Aqueous DSSCs were assembled using screen-printed TiO_2 semiconducting layers sensitized with an organic dye, $XY1b$. The redox couple was $TEMPO/TEMPO^+$ dissolved in aqueous $LiClO_4$ with MBI added as organic corrosion inhibitor. To improve the accessibility of the photoanodes for the redox couple, the size of TiO_2 nanoparticles was varied. Further, this helps to add a scattering layer. In a second approach, the sealing method for the cells was adjusted. For instance, the distance between the working electrode and the counter electrode was tuned by using different sealant materials, such as hotmelt foils or UV glue, in order to allow short pathways for ion conduction. In this context, interactions of different sealant materials and the organic redox mediators have to be considered. The influence of the different

approaches on cell efficiency will be discussed.

DS 20.49 Wed 16:00 P3

Development of a Transport Layer for the Integration of a TiO2-based Photoanode on a Silicon Wafer for Solar Water Splitting — •Luisa Busch, Dennis Berends, and Kai Gehrke — DLR Institut für Vernetzte Energiesysteme, Oldenburg, Germany

Recently, Segev et al. [1] proposed a three-terminal hybrid photoelectrochemical (PEC) / photovoltaic (PV) device for improved solar spectrum utilization. The concept integrates a TiO2 photoanode on an IBC silicon wafer in tandem configuration. To overcome the rather large bandgap of TiO2, which still limits the absorption of the solar spectrum and therefore the efficiency of the PEC, a sub-stochiometric TiO2 layer is advantageous. However, contacting the two semiconductors directly would result in a high recombination of the free charge carriers and thus low currents in the cell, due to band mismatch. By adding a transport layer between the two materials, for example a tunnel recombination junction, an improved current flow can be achieved. Within this work, the development of such a transport layer is presented in order to integrate a sub-stochiometric TiO2 photoanode on a Si wafer. For this purpose, the optoelectronic properties of the two semiconductor materials are characterized to select a suitable transport layer material by simulating the band alignment with AFORS-HET. Based on these results, a possible transport layer is developed and integrated into the tandem structure for electrochemical characterization.

[1] G. Segev et al., In: *Nature materials*, 17(12):1115-1121, 2018. doi: 10.1038/s41563-018-0198-y

DS 20.50 Wed 16:00 P3

Hybrid thin film for H2 evolution applications — •Morgan Le Dû[1], Manuel Andree Reus[1], Kun Sun[1], Zerui Li[1], Cristiane Henschel[2], Andre Laschewsky[2,3], Sigird Bernstorff[4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Universität Potsdam, Institut für Chemie, 14476 Potsdam-Golm — [3]Fraunhofer Institut für Angewandte Polymerforschung, 14476 Postdam-Golm — [4]Elettra-Sincrotrone Trieste, Basovizza, 34149 Trieste, Italy — [5]MLZ, TU München, 85748 Garching

Photocatalysis via water splitting reaction is a way to implement the sun to produce hydrogen-based energy. Recently, Pt loaded graphitic carbon nitride (g-CN) has been found has a promising photocatalyst for H2 evolution under visible light. The aim of this work is to bring this material in a polymer thin film configuration to make it suitable for industrial purposes. Poly(N-isopropylacrylamide) exhibits good swelling capacity of water vapor and seems to be suitable for such a hybrid thin film system. A new isomer of PNIPAM, poly(N-vinylisobutyramide) (PNVIBAM) raised our attention due to its higher lower critical solution temperature (LCST) in aqueous solution ($\approx 39°C$) which makes it more stable in ambient environment. Spray coating has been chosen to be the deposition technique of PNVIBAM/g-CN/Pt hybrid films. A comparative study of the photocatalyst concentrations is presented. Grazing incident small angle x-ray scattering is the main tool of this work. G-CN/Pt blended polymer films structure is analysed under light irradiation condition.

DS 20.51 Wed 16:00 P3

Fabrication and electrochemical characterization of 2D membranes — •Yossarian Liebsch — Universität Duisburg-Essen, AG Schleberger, Germany

Membranes are critical components in widely used industrial and technical processes, *e.g.*, water filtration, desalination and energy storage and conversion. With their extreme thinness of only a few angstrom, two-dimensional (2D) materials have the potential to be used as highly efficient membranes, possibly outperforming conventional membranes by orders of magnitude. We fabricated two different types of 2D membranes: Membranes made of commercially available CVD-grown graphene and membranes made of self grown CVD MoS_2. The membranes were made by transferring the 2D material onto a $3\,\mu$m micropore. Subsequently the membranes were plasma etched (graphene) or irradiated by highly charged ions (MoS_2) in order to create nanopores. Raman and photoluminescence spectroscopy was used to analyse the membranes in terms of doping, stress and defects density. Additionally an electrochemical characterization of the membranes was done in a custom build membrane potential measurement stand. In case of the graphene membranes the measured membrane potentials were in good agreement to the well-known Theorell-Meyer-Sievers Theory. However for the MoS_2 membranes no potential could yet be measured. In upcoming experiments with this electrochemical cell we aim to investigate the correlations between the pore creation mechanisms and intrinsic membrane properties like pore size, pore chemistry and surface charge density.

DS 20.52 Wed 16:00 P3

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

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

DS 21: Layer Deposition (ALD, MBE, Sputtering, ...)

Time: Thursday 9:30–10:30 Location: H14

DS 21.1 Thu 9:30 H14

Surface-Diffusion Control Enables Tailored-Aspect-Ratio Nanostructures in Area-Selective Atomic Layer Deposition — •Philip Klement[1], Daniel Anders[1], Lukas Gümbel[1], Michele Bastianello[1], Fabian Michel[1], Jörg Schörmann[1], Matthias T. Elm[1,2], Christian Heiliger[3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I & Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Institute of Physical Chemistry, Justus Liebig University Giessen, Giessen, Germany — [3]Institute of Theoretical Physics & Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany

Area-selective atomic layer deposition is a key technology for modern microelectronics as it enables material deposition only in specific areas. Typically, the selectivity originates from surface modifications of the substrate that allow or block precursor adsorption. The control of the deposition process currently remains a major challenge as the selectivity of the no-growth areas is lost quickly. Here, we show that surface modifications of the substrate strongly manipulate the surface diffusion. The selective deposition of TiO2 on poly (methyl methacrylate) and SiO2 yields localized nanostructures with tailored aspect ratios. Controlling the surface diffusion allows to tune such nanostructures as it boosts the growth rate at the interface of the growth and no-growth areas. Kinetic Monte-Carlo calculations reveal that species move from high to low diffusion areas.

DS 21.2 Thu 9:45 H14

Molecular-beam epitaxy of Cd- and Nb-containing Bi_xSe_y-based compounds for novel topological materials — •Christoph Ringkamp[1], Abdur Rehman Jalil[2], Erik Zimmermann[1], Peter Schüffelgen[1], Thomas Schäpers[1], Gregor Mussler[1], and Detlev Grützmacher[1] — [1]PGI-9, Forschungszentrum Jülich — [2]PGI-10, Forschungszentrum Jülich

Topological insulators (TIs) have gained a lot of interest in recent years because of their unique topologically protected surface states. Prominent examples of 3-dimensional topological insulators are Bi_2Te_3, Sb_2Te_3, and Bi_2Se_3 and alloys thereof. The combination of TI with superconductors and using the proximity effect to induce superconductivity in the TI is of fundamental interest in physics and may direct a possible avenue towards novel applications in the field of quantum computation. Here the successful deposition of Cd- and Nb-containing Bi_xSe_y

films by molecular beam epitaxy is reported. Carefully adjusting the growth parameter, single-crystal $CdBi_2Se_4$ and $(BiSe)_{1.10}NbSe_2$ thin films have been grown on sapphire substrates. For both materials, transmission electron microscopy images reveal the expected stacking sequences of atomic layers within the deposited films, indicating the presence of the anticipated stoichiometry. First data of the electrical transport of $(BiSe)_{1.10}NbSe_2$, films show superconducting behavior with a transition temperature of 0.4 K.

DS 21.3 Thu 10:00 H14

Growth and Characterization of Epitaxial (Cr1-xMnx)2GaC MAX Phase Thin Films by Pulsed Laser Deposition — •Ivan Tarasov, Hanna Pazniak, Michael Farle, and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Due to their nanolaminated structure, tunable chemistry, and high oxidation resistance, MAX phases (where M is an early transition metal, A is a main group element, and X is carbon or nitrogen) are interesting materials for a wide variety of applications. The partial substitution of M atoms is one of the ways to tailor their properties to specific applications. In this study, we grow (Cr1-xMnx)2GaC MAX phase films to fine-tune their magnetic response by stoichiometry variations for x = 0-1. High-quality epitaxial (Cr1-xMnx)2GaC MAX phase films (thickness 30 * 100 nm) are synthesized by pulsed laser deposition on MgO (111) substrates using (Mn50Cr50)66Ga34, Mn0.66Ga0.34, Cr66Ga34 and C targets. The combination of structural and morphological characterization reveals a strong competition between the (Cr1-xMnx)2GaC MAX phase and (Cr1-xMnx)3GaC, (Cr1-xMnx)3Ga phases. We suppress the formation of side phases by variation of the growth temperature and the formation of seed layers. Vibrating sample magnetometry of the MAX phase reveals increasing magnetization and ordering temperature with increasing Mn content. Funding by the Deutsche Forschungs*gemeinschaft (DFG) within CRC/TRR 270, project B02 (Project-ID 405553726) is gratefully acknowledged.

DS 21.4 Thu 10:15 H14

Optical Quantizing Structures in Al2O3/TiO2 Heterostructures by Plasma Enhanced Atomic Layer Deposition (PEALD) — •Pallabi Paul[1,2] and Adriana Szeghalmi[1,2] — [1]Friedrich Schiller University Jena, Germany — [2]Fraunhofer Institute for Applied Optics and Precision Engineering, Jena, Germany

Atomically thin heterostructures are promising candidates for various optoelectronic and photonic applications. Here we present on the properties of Al2O3/TiO2 nano-composites grown by PEALD. The growth, dispersion relation, optical bandgap and composition of such structures are systematically studied by means of UV/VIS spectrophotometry, ellipsometry, XRR, STEM, and XPS techniques. The refractive index and the indirect bandgap of the heterostructures depend on the ratio of the two oxides, while the bandgap is very sensitive to the thicknesses of the barrier and quantum well layers. A large blue shift of the absorption edge from 400 nm to 320 nm is obtained by changing the TiO2 (quantum well) thickness from 2 nm to 0.1 nm. PEALD unfolds the possibility of achieving optical quantizing effects within complex heterostructures enabling control of their structures down to atomic scale. Selected compositions are identified for applications in antireflection coatings at 355 nm wavelength. Interference multilayers of TiO2/Al2O3 composites as high refractive index material and SiO2 as the low refractive index show very low reflectance and optical losses at 355 nm wavelength with transmittance values of approximately 99%. Such heterostructures overcome the limitations of the low bandgap dielectric TiO2 for optical applications in the UV spectral range.

DS 22: 2D Materials 8 (joint session DS/CPP)

Time: Thursday 9:30–11:30 Location: H17

DS 22.1 Thu 9:30 H17

Calculation of Elastic Properties in Monolayer Covalent-Organic Frameworks — •David Bodesheim[1], Antonios Raptakis[1], Jonathan Heinze[1], Arezoo Dianat[1], Robert Biele[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]TU Dresden, Dresden, Germany — [2]FSU Jena, Jena, Germany

Covalent-Organic Frameworks (COFs) are crystalline porous materials that are based on organic monomeric units, so called building blocks. Through recent experimental progress, mono- and few-layer COF materials have been synthesized, providing a new class of 2D materials.[1,2] From a computational point of view, however, accurately calculating properties of these materials is demanding as their unit cells are usually very big. In this work, we calculate elastic properties for a multitude of 2D COFs in a high-throughput manner. The calculations are based on classical force-fields and are compared with higher level of theory like density functional based tight binding (DFTB). We show how force-fields can be very useful for mechanical property calculation, how their accuracy can be improved, and typical fallacies for 2D COFs. Furthermore, we introduce models to predict mechanical properties from the properties of their monomeric building blocks.[3] This paves the way for accurate multiscale modeling, high-throughput calculations, and materials design with properties on demand.

[1] A. Ortega-Guerrero, et al. ACS Appl. Mater. Interfaces, 13, 22, 26411-26420 (2021).
[3] Z. Wang, et al., Nat. Synth., 1, 69-76 (2022).
[3] A. Raptakis, et al. Nanoscale, 13, 1077 (2021).

DS 22.2 Thu 9:45 H17

Light-Matter Interaction in 2D Polar Metals — •Margaux Lassaunière[1], Wen He[2], Katharina Nisi[1], Shruti Subramanian[3], Siavash Rajabpour[3], Alexander Vera[3], Nathalie Briggs[3], Su Ying Quek[2], Joshua Robinson[3], and Ursula Wurstbauer[1] — [1]Institut of Physics, Münster University, Germany — [2]Department of Physics, National University of Singapore, Singapore — [3]MatSE; Center for 2DLM; ATOMIC; 2D Crystal Consort.; Penn State University, USA

Understanding and controlling the light-matter interaction in thin metal films is of high technological relevance. Here, we study the linear optical response of atomically thin 2D gallium, 2D indium as well as their alloys embedded in half-van der Waals heterostructures by spectroscopic imaging ellipsometry. The thin films are prepared via confinement heteroepitaxy (Chet). In a systematic study of the dielectric functions, we separate free and bound electron contributions to the optical response, with the latter pointing towards the existence of thickness-dependent quantum confinement phenomena and epsilon near zero (ENZ) behaviour [1]. The resonance energies of the observed ENZ behaviour are dependent on the number of atomic metal layers, materials, and alloying [2]. Their tunability makes 2D polar metals attractive for quantum engineered metal films, tunable (quantum-)plasmonics and nano-photonics.

[1] K. Nisi et al. Adv. Mater. 2021, 2104265
[2] S. Rajabpour et al. Adv. Funct. Mater. 2020, 2005977

DS 22.3 Thu 10:00 H17

Layer dependent anisotropic dielectric function of the magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Margaux Lassaunière[1], Julian Klein[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA

The van der Waals (vdW) material CrSBr is a 2D magnetic semiconductor with ferromagnetic ordering within each layer. Adjacent layers, however, are coupled antiferromagnetically. As a vdw semiconductor with a direct band gap, the light matter interaction is determined by strong excitonic resonances that are highly anisotropic in the crystal plane. We experimentally determine the complex dielectric function in the near infrared to visible regime along the two main crystal directions by spectroscopic imaging ellipsometry (SIE) measurements and regression analysis to a multilayer model. Unlike other vdW semiconductors such as MoS2 or WSe2 [1], the rich excitonic signatures in the dielectric function are highly anisotropic and show only minor distinct dependence on the number of layers. Even more striking, we find that the excitonic resonance are better pronounced for multilayer compared to monolayer CrSBr with significantly reduced line-width even at room temperature. [1] Wurstbauer et al. J. Phys. D: Appl. Phys. 50, 173001 (2017).

DS 22.4 Thu 10:15 H17

Tracing the Superconducting Phase Transition in Atomically Thin 2D Polar Gallium by Transport and Spectroscopic Ellipsometry — •Jakob Henz[1], Margaux Lassunière[1], Pierre-Maurice Piel[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua Robinson[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

Half van der Waals 2D polar metals are a novel class of 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms such as gallium or indium are intercalated between graphene and a silicon carbide substrate. This results in large area, environmentally stable, 2D metals with a bonding gradient in z-direction ranging from covalent over metallic to vdW within only two to three atomic layers. The materials feature interesting properties such as superconductivity[1] and a large plasmonic response in the visible range[2]. 2D gallium is studied by temperature dependent spectroscopic ellipsometry and transport measurements down to below 1K. We extract the dielectric function in the visible to near infrared range with a special focus on signatures across the phase transition from metallic to superconducting behavior unambiguously identified from the abrupt drop in the temperature dependent sheet resistance at the transition temperature T_C of about 3.5 K.

1 S. Rajabpour et al., Adv. Mater. 2104265 (2021)
2 Nisi et al., Adv. Funct. Mater. 2005977, 1-11 (2020)

DS 22.5 Thu 10:30 H17

Epitaxial growth of $Fe_{5-x}GeTe_2$ films with a Curie temperature above 300 K on graphene — Hua Lv[1], Jens Herfort[1], Jürgen Schubert[2], Michael Hanke[1], Manfred Ramsteiner[1], and •Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Germany

Synthesis of magnetic 2D materials exhibiting transition temperatures at or above 300 K is a crucial step towards the development of ultra-compact spintronic devices. Here, we report our recent progress on epitaxial growth of the 2D ferromagnet $Fe_{5-x}GeTe_2$ via MBE on graphene on SiC(0001). Thin films with a thickness of about 10 nm and different Fe concentrations were studied. Characterization performed with methods such as in-situ RHEED and grazing incidence X-ray diffraction confirmed the formation of epitaxial layers with good crystalline quality. Magneto-transport measurements and SQUID magnetometry were employed to assess the electrical and magnetic properties. They reveal that the MBE-grown $Fe_{5-x}GeTe_2$ exhibits a metallic behavior for all investigated Fe concentrations. In addition, composition-dependent magnetic anisotropies and Curie temperatures (T_C) were deduced. For the Fe content close to 5, a predominant easy out-of-plane orientation and T_C well above 300 K were measured. These results are relevant for the further development of wafer-scale fabrication of magnetic 2D materials aiming at the realization of multifunctional, atomically thin devices.

DS 22.6 Thu 10:45 H17

Antisymmetric magnetoresistance in a Fe_3GeTe_2-Fe_3GeTe_2 van der Waals ferromagnetic homojunction — •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, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

The emergence of novel two-dimensional (2D) magnetic van der Waals (vdW) materials have breathed new life into the field of spintronics. The weak vdW interaction between layers of strong covalent bonds enables the exfoliation of these materials down to monolayers. Furthermore, vdW heterostructures can easily be fabricated by stacking them on top of each other like LEGO blocks, bringing a platform for novel spintronic devices. Here, we report an antisymmetric magnetoresistance (MR) in an Fe3GeTe2- Fe3GeTe2 (FGT) vdW homojunction. We attribute it to eddy currents emerging at the interface of the antiparallel, perpendicular-to-plane magnetized FGT flakes, due to the different sign of the anomalous Hall effect in both flakes. These eddy currents perturb the measured longitudinal resistance, resulting in the observed antisymmetry. Such an interpretation is supported by the observation of a sign change of the MR when measuring the voltage drop along the opposite edges of the transport channel . This work highlights the potential for new spintronic applications using vdW ferromagnets.

DS 22.7 Thu 11:00 H17

Charge-transfer stabilization, modulation doping, and CDW phase in layered ferecrystal heterostructures — •Fabian Göhler[1], Shrinidhi Ramasubramanian[1], Sanam K. Rajak[1], Niels Rösch[1], Adrian Schütze[1], Susanne Wolff[1], Marisa Choffel[2], Dmitri L. M. Cordova[2], David C. Johnson[2], and Thomas Seyller[1] — [1]Chemitz University of Technology, 09126 Chemnitz, Germany — [2]University of Oregon, Eugene 97403, USA

A virtually unlimited number of metastable, layered heterostructures - called *ferecrystals* due to the non-epitaxial alignment between layers - can be grown via the self-assembly of layered amorphous precursors. [1] In this contribution, we want to highlight recent investigations on the electronic structure and interlayer interactions in several series of compounds using photoemission spectroscopy (PES).

In the Bi-Mo-Se system, the formation of the metallic 1T-polytype of $MoSe_2$ is aided by charge transfer from rock-salt structured BiSe. By systematically stacking BiSe, Bi_2Se_3, and $MoSe_2$, the mechanisms which stabilize these structures can be understood. [2]

Compounds prepared from PbSe and VSe_2 layers show charge transfer between layers as well, allowing to tune transport properties via modulation doping. Additionally, the emergence of a charge density wave in the VSe_2 layers has been reported below 100 K [3], and was investigated by angle-resolved PES.

[1] Esters et al., *Angew. Chem. Int. Ed.* **54**, 1130 (2015).
[2] Göhler et al., *J. Phys. Chem. C* **125**, 9469 (2021).
[3] Cordova et al., *Chem. Mater.* **31**, 8473 (2019).

DS 22.8 Thu 11:15 H17

Impact of opto-electronic measurements on the properties of hexagonal boron nitride as a dielectric — •Jo Bertram[1], Luca Kotewitz[1], Manfred Ersfeld[1], Frank Volmer[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Hexagonal boron nitride (hBN) serves as an atomically flat, insulating substrate for a large variety of 2D heterostructures. However, recent opto-electronic experiments showed that optically triggered leakage currents passing through hBN pose a serious bottleneck for reliable gating of 2D semiconductors [1]. Motivated by these observations, we report on photo-induced charge transport through hBN in graphite-hBN-graphite devices. Furthermore, we examine the impact of illuminating hBN employed as a gate dielectric on the charge carrier density of graphene Hall bar devices. Our results indicate that hBN exhibits optically active electronic states, which partially screen the gate electric field under light illumination. Interestingly, we observe a strong asymmetry of this effect for positive and negative electric fields showing that hBN does not behave as an ideal dielectric within the plate capacitor model especially in opto-electronic experiments.

[1] F. Volmer et al., Phys. Status Solidi RRL 14, 2000298 (2020)

DS 23: Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...)

Time: Thursday 10:45–12:15 Location: H14

DS 23.1 Thu 10:45 H14

Raman characterisation of composite thin films of PEDOT:PSS and Cu2ZnSnS4 nanocrystals — •Yevhenii Havryliuk[1,2,3], Volodymyr Dzhagan[3], Oleksandr Selyshchev[1,2], and Dietrich R.T. Zahn[1,2] — [1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures, and Integration of Nanomembranes (MAIN), Chemnitz, Germany — [3]V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine, Kyiv, Ukraine

The increasing demand for renewable energy sources powers the high research interest in the fields of photovoltaics and thermoelectrics. One of the materials promising in these fields are Cu2ZnSnS4 (CZTS) family compounds. CZTS nanocrystals (NCs) for third generation photovoltaics can be obtained by low-temperature "green" colloidal synthesis. Another material widely studied especially for thermoelectric applications is PEDOT:PSS. Usually these two materials are used as separate layers in devices. However, using them in a composite layer probably can reveal even more interesting properties. Therefore, we investigated such composite films with different polymer/NC ratios. Raman spectroscopy was used as a main characterization method. We detected the modification of the structure of PEDOT:PSS films upon incorporation of NCs and found that the formation of the CZTS NCs films using a drop-casting method occurs differently in the presence of even a small amount of PEDOT:PSS. The change in the stability of the PEDOT:PSS/CZTS composite under intense laser irradiation, in comparison with the pure components, was also investigated.

DS 23.2 Thu 11:00 H14

dielectric function of Al(1-x)ScxN obtained by spectroscopic ellipsometry. — •Younes Slimi[1], Rebecca Petrich[1], Rüdiger Schmidt-Grund[1], Hauke-Lars Honig[2], Christina Helm[3], Heike Bartsch[3], Jens Müller[3], Peter Schaaf[2], and Stefan Krischok[1] — [1]Fachgebiet Technische Physik I, IMN Macro Nano, Technische Universität Ilmenau, 98693 Ilmenau — [2]Fachgebiet Werkstoffe der Elektrotechnik, Institut für Werkstofftechnik und Institut für Mikro-und Nanotechnologien MacroNano, Technische Universität Ilmenau, 98693 Ilmenau — [3]Fachgebiet Elektroniktechnologie, Technische Universität Ilmenau, IMN Macro Nano, 98693 Ilmenau

Scandium Aluminum Nitride alloy (ScxAl1-xN) thin films were prepared via the sputtering technique. The samples then were measured by spectroscopic ellipsometry (SE) and analysed to determine the sample's dielectric function (DE) by means of numeric b-spline and line shape model dielectric functions. We found a redshift of the bandgap (Eg) and an increasing refractive index with increasing Sc content. As AlN is hexagonal and ScN cubic, the birefringence also reduces when Sc is incorporated into the alloy. Therefore, the samples were measured with XRD and EDX to determine the crystal structure and lattice constant as a function of Sc percentage.

DS 23.3 Thu 11:15 H14

Analysis of CVD coatings with Raman spectroscopy — •Maximilian von Roeder, Peter J. Klar, and Sangam Chatterjee — Institute of Experimental Physics I, Giessen, Germany

The interphase between fibre and matrix is an important component in the preparation of ceramic matrix composites. The understanding of the nature of the coating is crucial for the optimization of CMC materials. Chemical vapour infiltration is the most frequent method of fibre coating. Homogenity, low error density and controlled thickness are the key properties that the coating has to satisfy. Most characterization methods for the coating are very local probes. We applied rough Raman mapping measurements together with principal component analysis to get a broader picture for a larger sample. We studied SiC Hi-Nicalon S fibres with BN/SiC and C coating prepared by chemical vapour infiltration. With a data filtering algorithm to erase the raman spectra of the background we were able to obtain a colour coded maps of the samples. We tested this method with different samples where we introduced errors of different magnitude to determine the sensitivity of the approach. This method provides a quick and easy way to examine a sample with the extensions up to a few centimeters. In this fashion it is possible to study a larger fraction of a prepared material which leads to a higher reliability in quality control.

DS 23.4 Thu 11:30 H14

Time-resolved femtosecond ellipsometry — •Shirly Espinoza — ELI Beamlines, Institute of Physics, Czech Academy of Science, Prague, Czech Republic

The ellipsometry technique is well extend for the study of thin film material. Thanks to femtosecond pulse lasers, we developed a time-resolved femtosecond ellipsometry technique, where a pump beam from any wavelength between 200 nm and 2000 nm excite the material and second pulse, the probe beam, with a continuous spectrum from 350 nm * 750 nm measure the dielectric function of the material. The pump and the probe beam can be separated in time from femtoseconds until nanoseconds generating a time-scan of the relaxation of the material. The time-resolved ellipsometry technique is available to the scientific community at the user-oriented infrastructure ELI Beamlines located few kilometers from Prague, Czech Republic. Examples of successful experiments will be presented and the details of how to apply for beamtime will be shared.

DS 23.5 Thu 11:45 H14

Chalcogenides for Photonic Applications in the Visible — •Felix Hoff[1], Carl-Friedrich Schoen[1], Maximilian Mueller[1], Yiming Zhou[1], Peter Kerres[1], Häser Maria[1], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Juelich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]PGI 10 (Green IT), Forschungszentrum Juelich GmbH

Due to its large bandgap, the chalcogenide phase-change material (PCM) Sb_2S_3 is interesting for photonic applications, such as photonic switches in the visible range. Recent publications report contradictory findings concerning the switching speed. Since this property is decisive for many applications, it is important to better understand the crystallization process. To understand glass dynamics and crystallization kinetics, calorimetric measurements were performed. In addition, the optical properties were measured by optical spectroscopy and Ellipsometry. Supporting density functional theory (DFT) calculations are used and a comparison with typical PCMs is made. Sb_2S_3 has significant optical contrast in the visible spectral range, but lower maximum contrast than typical PCMs. It has been shown that crystallization takes significantly longer and has a broader stochastic distribution than for typical PCMs. Furthermore, crystallization occurs from the undercooled liquid phase for a range of heating rates which span over six orders of magnitude, so the glass transition could be studied. Our observations can be explained by the covalent bonding of Sb_2S_3. They can be understood in the context of a quantum mechanical map, which can be utilized to design materials for photonic applications.

DS 23.6 Thu 12:00 H14

IR dual-comb polarimetry of a nanofiber scaffold — •Karsten Hinrichs[1], Brianna Blevins[2,3], Andreas Furchner[4], Nataraja Sekhar Yadavalli[2,3], Sergiy Minko[2,3,5], Raphael Horvath[6], and Markus Mangold[6] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Nanostructured Materials Laboratory, The University of Georgia — [3]Department of Chemistry, The University of Georgia — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Division Energy and Information, Schwarzschildstraße 8, 12489 Berlin, Germany — [5]Department of Textile, Fiber, and Polymer Sciences, The University of Georgia, Athens, Georgia 30602, United States — [6]IRsweep AG, Laubisruetistrasse 44, 8712 Staefa, Switzerland

In this study the transmission properties of an anisotropic nanofiber scaffold are investigated non-invasively under ambient conditions by IR dual-comb polarimetry (DCP). Good agreement between DCP and classical FTIR polarimetry is found for amplitude and phase measurements at various azimuthal sample rotations, proving DCP as a new method for the study of such anisotropic samples in very short measurement times. A spectral information in the range of 1200 cm-1 to 1300 cm-1 can be achieved in 0.065 ms at 1.4 cm-1 spectral resolution showing the potential for imaging applications, time resolved studies and hyperspectral spectroscopy of anisotropic samples. We acknowledge financial support by the EU through EFRE 1.8/13 and the Horizon 2020 grant 820419 and by the BMBF through CatLab (03EW0015A).

DS 24: 2D Materials 9 (joint session HL/CPP/DS)

Time: Thursday 11:15–12:15 Location: H36

DS 24.1 Thu 11:15 H36

Generating extreme electric fields in 1 2D materials by dual ionic gating — •Benjamin Isaac Weintrub[1], Yu-Ling Hsieh[1,2], Jan N. Kirchhof[1], and Kirill I. Bolotin[1] — [1]Department of Physics, Freie Universität Berlin, Berlin, Germany — [2]Department of Mechanical Engineering, National Central University, Taoyuan City, Taiwan

We demonstrate a new type of dual gate transistor to induce record electric fields through two-dimensional materials (2DMs). At the heart of this device is a 2DM suspended between two volumes of ionic liquid (IL) with independently controlled potentials. The potential difference between the ILs falls across an ultrathin layer consisting of the 2DM and the electrical double layers above and below it, thereby producing an intense electric field across the 2DM. We determine the field strength via i) electrical transport measurements and ii) direct measurements of electrochemical potentials of the ILs using semiconducting 2DM, WSe2. The field strength across a bilayer WSe2 sample reaches ~2.5 V/nm, the largest static electric field through the bulk of any electronic device to date. Additionally, we create electric fields strong enough to close the bandgap of 3-layer and 4-layer WSe2 (~1.4 V/nm and ~0.9 V/nm respectively). Our approach grants access to previously-inaccessible phenomena occurring in ultrastrong electric fields.

DS 24.2 Thu 11:30 H36

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova — HORIBA Jobin Yvon GmbH, Neuhofstr. 9, Bensheim 64625, Germany

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

DS 24.3 Thu 11:45 H36

Defects in 2D WS_2 monolayers — Aswin Asaithambi[1], Roland Kozubek[1], Francesco Reale[2], Erik Pollmann[1], Marcel Zöllner[1], Cecilia Mattevi[2], Marika Schleberger[1], Axel Lorke[1], and •Günther Prinz[1] — [1]Fakultät für Physik und CENIDE, Universität Duisburg-Essen, Germany — [2]Department of Materials, Imperial College London, UK

In this presentation, we report about optical characterization and manipulation of defects in tungsten disulfide (WS_2) monolayers. WS_2 is one prominent member of the 2D transition metal dichalcogenides (TMDC). In these materials, defects and adsorbates can easily modify e.g., conductivity, optical properties, or even create single photon emitters. For this study we used high quality WS_2 CVD-grown monolayers to purposely introduce defects via irradiating them with Xe^{30+} ions with different fluences [1]. Low temperature photoluminescence (PL) spectra of these irradiated WS_2 monolayers show two defect related broad bands, beside the excitonic contribution. By exposing these flakes to laser light with powers up to 1.5mW, the intensity of these two PL bands can be reduced. By comparing the intensity of the excitonic contribution before and after this laser processing, we don't observe an increase in intensity, leading us to conclude, that the defects aren't getting healed. If the samples are heated to room temperature, the defect luminescence recovers. To interpret our observation, we suggest that the defects might be attributed to vacancy defects together with adsorbates at different defect sites.

[1] A. Asaithambi et al., Phys. Status Solidi RRL 2021, 15, 2000466

DS 24.4 Thu 12:00 H36

Large perpendicular field in bilayer TMD via hybrid molecular gating — •Sviatoslav Kovalchuk[1], Abhijeet Kumar[1], Simon Pessel[1], Kyrylo Greben[1], Dominik Christiansen[2], Malte Selig[2], Andreas Knorr[2], and Kirill Bolotin[1] — [1]Department of Physics, Quantum Nanoelectronics of 2D Materials, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We consider structures in which bilayer TMDs are sandwiched between a layer of molecules and Si gate. We show that these structure allow increasing, by a factor of 2, maximum electric field achievable in this 2D material. This in turn, allows reaching electric field >0.2 V/nm. In MOS2 this is sufficient to bring interlayer excitons IX into resonance with either A or B intralayer excitons. We study coupling between these excitons, and give an outlook on the new technique to achieve large perpendicular electric fields detectable in optical measurements.

DS 25: Transport Properties

Time: Thursday 15:00–16:00 Location: H14

DS 25.1 Thu 15:00 H14

Visualization of metallic filament formation in rare-earth nickelates via optical microscopy — •Theodor Luibrand[1], Stefan Guénon[1], Farnaz Tahouni-Bonab[1], Javier del Valle[2], Claribel Domínguez[2], Willem Rischau[2], Lucia Varbaro[2], Stefano Gariglio[2], Rodolfo Rocco[3], Soumen Bag[3], Marcelo Rozenberg[3], Jean-Marc Triscone[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) an LISA$^+$, Universität Tübingen, 72076 Tübingen, Germany — [2]Department of Quantum Matter Physics, Université de Genève, 1211 Geneva, Switzerland — [3]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France

In recent years, there has been growing interest in resistive switching in strongly correlated materials. Resistive switching is at the core of memristive devices, which are considered as crucial elements in the emerging field of neuromorphic computing. However, in many systems, the details of the resistive switching mechanisms are elusive. We investigated the resistive switching of two types of rare-earth nickelate ($NdNiO_3$ and $SmNiO_3$) thin film devices. Both materials undergo insulator-to-metal transitions (IMT) from low-temperature antiferromagnetic or paramagnetic insulating to high-temperature paramagnetic metallic phases. Current-voltage characteristics acquired at device temperatures near the IMT show jumps towards lower voltages indicating resistive switching. We find that these events are accompanied by the formation of spatially confined conducting filaments, which is revealed by a change in reflectivity in optical images.

DS 25.2 Thu 15:15 H14

Towards ultraclean correlated metal $CaVO_3$ - Electric Transport Measurements — •Mahni Müller[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and Saskia F. Fischer[1] — [1]Novel Materials Group, HU Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA. — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany

High-performance and cost-effective transparent materials are in great demand in the optoelectronic industry. The enhancement of the carrier effective mass through strong electron-electron interactions in cor-

related metals is a promising approach to achieve both high-optical transparency and high-electrical conductivity [1].

In this work we study the electric transport characteristics of $CaVO_3$ films with a thickness of 55 nm grown on LAO substrates. The films were deposited by hybrid molecular beam epitaxy with different partial pressures of the metalorganic vanadium oxytriisopropoxide precursor. Calcium was supplied through a solid state effusion cell. The optimal growth window estimated by X-ray diffraction was narrowed down by residual-resistance ratio (*RRR*) measurements. Temperature dependent resistivity and hall measurements were performed between 4.2 K and 300 K. The *RRR* was tripled compared to previous substrate [2]. Furthermore, the films with highest $RRR \approx 98$ showed an increase of mobility with decreasing temperature with over 2000 $\frac{\text{cm}}{\text{V}\cdot\text{s}}$ at 4.2 K.

[1] Zhang, Lei, *et al.*; Nature materials **15.2**, 204-210 (2016).

[2] Eaton, Craig, *et al.*; J. Vac. Sci. Technol. **35.6**, 061510, (2017).

DS 25.3 Thu 15:30 H14

Electro-Thermal Resistive Switching at the Insulator to Metal Transition in Strongly Correlated Materials — •Stefan Guénon[1], Matthias Lange[1], Yoav Kalcheim[2,3], Theodor Luibrand[1], Farnaz Tahouni[1], Reinhold Kleiner[1], Ivan K Schuller[2], and Dieter Koelle[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, 72076 Tübingen, Germany — [2]Department of Physics and Center for Advanced Nanoscience, University of California - San Diego La Jolla, CA 92093, USA — [3]Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Technion City, 32000 Haifa, Israel

Electro-thermal (Joule-heating driven) resistive switching devices are investigated in the emerging field of neuromorphic computing. In a biomimetic approach, the memristive properties of such devices are used to emulate neurons and synapses. This talk explains how the considerable resistance change at the insulator-to-metal transition leads to electro-thermal instability. A metallic filament forms above a certain threshold current due to current and temperature redistribution if a device is electrically biased in this unstable temperature regime. We will complement the explanation with experimental results from microscopic studies on V_2O_3-devices, in which photomicrographs were acquired during filament formation. Further, we will discuss how additional device properties like thermal hysteresis or structural phase separation affect electro-thermal resistive switching. The U.S. Department of Energy supported this work under Award # DE-SC0019273.

DS 25.4 Thu 15:45 H14

Parallel field magnetoconductance in epitaxial bismuth quantum films — •Julian Koch[1], Doaa Abdelbarey[2], Philipp Kröger[2], Priyanka Yogi[2], Christoph Tegenkamp[1], and Herbert Pfnür[2] — [1]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover

The magnetoconductance (MC) of epitaxial Bi films on Si(111) (thickness 20-100 bilayers) was measured at $T = 9$ K in magnetic fields oriented in-plane parallel and perpendicular to the electric dc current I. Contributions to MC by weak antilocalization (WAL), by weak localization (WL) as well as by diffuse scattering were identified, which all turned out to be independent of the angle between B and I. In addition, only for $B \perp I$ a contribution to MC was found that *increases* with increasing B and is, to first approximation, $\propto B^2$. It is ascribed to ballistic scattering between the Rashba-split interfaces that allow Umklapp scattering without spin flip.

At small thicknesses the MC curves are dominated by WAL originating from the surface/interface states. However, the coupling between the interfaces, necessary for the observation of WAL in an in-plane B-field, happens through quantized bulk states instead of tunneling. Moreover, the admixing of the quantized bulk states with increasing film thickness not only increases diffuse scattering, but also modifies the WAL component, effectively introducing a WL-like component, above 50 BL. Thus, our findings suggest an intriguing interplay in magnetotransport between 2D and quantized 3D states.

DS 26: Thin Oxides and Oxide Layers 2

Time: Thursday 16:15–17:15 Location: H14

DS 26.1 Thu 16:15 H14

Studying the differences of Ga2O3 grown by conventional molecular-beam epitaxy (MBE) and suboxide MBE (S-MBE) — •Sushma Raghuvansy[1], Justin A. Bich[1], Tjark Liestmann[1], Jonathan McCandless[2], Manuel Alonso-Orts[1], Darrell G. Schlom[3], Martin Eickhoff[1], and Patrick Vogt[1,3] — [1]Institute of Solid-State Physics, Bremen University, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]School of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853, USA — [3]Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA

The growth of Ga2O3 by conventional MBE, i.e., when supplying elemental Ga and active O, is limited by the formation and subsequent desorption of its volatile suboxide, Ga2O. During suboxide MBE (S-MBE), a recently developed new MBE variant, suboxides (here: Ga2O) are supplied during growth, bypassing the reaction limiting steps experienced during conventional Ga2O3 MBE growth by conventional MBE, and extending its kinetic and thermodynamic limits. S-MBE enables the synthesis of Ga2O3 at much higher growth rates (> 1 μm h-1) and displays improved crystallinity and surface morphology compared with Ga2O3 thin films grown by conventional MBE.

This talk presents a direct comparison of Ga2O3 thin films grown by conventional MBE versus Ga2O3 thin films grown by S-MBE. We will show the impact of both MBE variants on the crystallinity and surface morphology of Ga2O3/Al2O3 heterostructures.

DS 26.2 Thu 16:30 H14

Comparative Study of a Ga2O3 nucleation layer and its impact on Ga2O3 growth on Al2O3 by molecular beam epitaxy — •Alexander Karg, Adrian Messow, Manuel Alonso-Orts, Stephan Figge, Patrick Vogt, and Martin Eickhoff — Institute of Solid-State Physics, University Bremen, Bremen, Germany

Ga2O3 is a wide bandgap semiconductor and is seen as a promising candidate for e.g. future high-power electronics, and UV-detectors. The availability of single crystalline substrates makes the material attractive for device fabrication. Because of easier access, the majority of experiments were carried out by heteroepitaxy on e.g. Al2O3 substrates. In this study, the influence of the Al2O3 substrate on the nucleation and layer growth is investigated and compared with the use of a beta-Ga2O3 buffer layer to mimic homoepitaxial conditions. It was found that the effective Me to O ratio on the surface differs substantially and the amount of the available species (especially active oxygen) for growth could be estimated with respect to the different growth surfaces (0001) Al2O3 and (-201) beta-Ga2O3. This study was transferred to In2O3 growth to determine the different oxidation efficacies of the cations Indium and Gallium. Furthermore, the influence of the plasma power on the nucleation behavior of Ga2O3 and In2O3 as well as its influence on the growth kinetics itself and the layer properties will be discussed.

DS 26.3 Thu 16:45 H14

The effect of post-growth annealing of titanium dioxide thin films prepared by a sol-gel process on the photocatalytic activity — •Lu He[1], Shuo Niu[1], Dietrich.R.T. Zahn[1,2], and Teresa I. Madeira[1,2] — [1]Technische Universität Chemnitz, Semiconductor Physics, D-09107 Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, 09107 Chemnitz, Germany

TiO2 thin films revealed competitive performance for photocatalytic applications[1,2]. Here, a set of TiO2 thin films are synthesized using a sol-gel process and spin coated on p-type Si(100) substrates with a native oxide layer. The as-deposited thin films are annealed at various temperatures from 400 to 800 °C for 3 hours in ambient conditions.

Characterization is performed using various methods[3] on phases (UV-Raman & X-Ray diffractometry), film thickness and optical constants (Spectroscopic ellipsometry), morphology(Atomic Force Microscopy). Photocatalytic results on photodegradation of acetone to CO2 are obtained in a self-designed gas (reactant)-solid (photocatalyst) reaction chamber. The decrease/increase of acetone/CO2 is mon-

itored via in-situ Fourier Transform Infrared Spectroscopy.

Quantitative data analysis is performed and correlated to indicate the effect of post annealing on the optical and structural properties of the titanium dioxide thin films and their photocatalytic activities.

1. Song,H et al, Conf. Lasers Electro-Optics,CLEO 2019
2. Nalajala et al, C.S.RSC Adv. 9 2019.
3. Gartner,M et al, Sol-Gel Sci. Technol. 2021

DS 26.4 Thu 17:00 H14

Oxidation behavior of SMART alloys and MAX phases materials and applicability in solar receivers. — •Leonardo Guimarães Leal Lealdini[1], Andrey Litnovsky[1,2], and Jesus Gonzalez-Julian[1,3] — [1]Forschungszentrum, Jülich GmbH, 52425 Jülich, Germany — [2]115409 Moscow, Russia — [3]Institute of Mineral Engineering, RWTH Aachen University, 52064 Aachen, Germany

In the concept of materials for high-temperature application, two types of are being investigated: SMART alloys and MAX phase materials. W-Cr-Y SMART alloys were first designed for future fusion power plants. Studies suggests that SMART alloy containing Cr and Y is capable of forming a Cr2O3 layer and maintaining it at 1273K which avoids the generation of tungsten oxide. MAX Phase materials are able to provide great properties like oxidation resistance at high temperatures. Cr2AlC and Ti2AlC are two MAX phases that, in initial studies, provided a good oxidation response. Studies showed that Cr2AlC MAX phase and W-Cr-Y SMART alloy when exposed to 1273K and in humid atmosphere present good resistance to oxidation. Both were capable of withstand more than 20 hours in these conditions with a gain of mass lower than 0.3g/cm2. The main objective of this research is to evaluate the feasibility of both MAX phase materials and propose a new W-Al-Y SMART alloy, using them as solar receivers in concentrated solar power plants.

DS 27: 2D Materials 10 (joint session HL/CPP/DS)

Time: Friday 9:30–12:00 Location: H36

DS 27.1 Fri 9:30 H36

THz conductivity of nanograined Bi2Te3 pellets with varying Te doping — •Ahana Bhattacharya[1], JeongWoo Han[1], Sepideh Izadi[2], Sarah Salloum[3], Stephan Schulz[3], Gabi Schierning[2], and Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Universität Bielefeld, Fakultät für Physik, 33615 Bielefeld, Germany — [3]Universität Duisburg-Essen, Fakultät für Chemie, 45141 Essen, Germany

The topological insulator Bi2Te3 hosts surface states with a high carrier mobility as back scattering of charge carriers is suppressed due to the spin-momentum locking. While in large crystals the electronic properties are dominated by the bulk states, hot-pressed pellets of nanograined Bi2Te3 offer a high surface-to-volume ratio, which provides a platform to exploit the surface carriers even in extended samples. Here we employ THz time-domain spectroscopy to disentangle the contribution of surface and bulk carriers to the transport properties. Even at room temperature the THz reflection is determined by characteristic features of the high-mobility surface carriers, i.e. Drude conductivity but also plasmonic contributions. The latter are caused by confinement of the surface carriers due to the mechanical structure of the sample. Variations of the Te content allows to shift the Fermi energy and thus strongly influences the resulting THz spectra.

DS 27.2 Fri 9:45 H36

Direct growth of monolayer MoS2 on nanostructured silicon waveguides — •A Kuppadakkath[1], E Najafidehaghani[2], Z Gan[2], A Tuniz[3], G Ngo[1], H Knopf[1], F Löchner[1], F Abtahi[1], T Bucher[1,5], S Shradha[1], T Käsebier[1], S Palomba[3], N Felde[4], P Paul[1], T Ullsperger[1], S Schröder[4], A Szeghalmi[1,4], T Pertsch[1,4], I Staude[1,5], U Zeitner[1,4], A George[2], A Turchanin[2], and F Eilenberger[1] — [1]Institute of Applied Physics (FSU), Jena, Germany — [2]Institute of Physical Chemistry (FSU), Jena, Germany — [3]Sydney Nano, Camperdown, Australia — [4]Fraunhofer IOF, Jena, Germany — [5]Institute of Solid State Physics (FSU), Jena, Germany

We report for the first time the direct growth of Molybdenum disulfide (MoS2) monolayers on nanostructured silicon-on-insulator waveguides. Our results indicate the possibility of utilizing the Chemical Vapour Deposition (CVD) on nanostructured photonic devices in a scalable process. Direct growth of 2D material on nanostructures rectifies many drawbacks of the transfer-based approaches. We show that the van der Waals materials grow conformally across the curves, edges, and the silicon-SiO2 interface of the waveguide structure. Here, the waveguide structure used as a growth substrate is complex not just in terms of its geometry but also due to the two materials (Si and SiO2) involved. A transfer-free method like this yields a novel approach for functionalizing nanostructured, integrated optical architectures with an optically active direct semiconductor.

DS 27.3 Fri 10:00 H36

Atomic layer deposition of ternary $MoWS_2$ — •Christian Tessarek, Tim Grieb, Andreas Rosenauer, and Martin Eickhoff — Institut für Festkörperphysik, Universität Bremen

Two-dimensional (2D) monolayers of binary molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) belong to the transition metal dichalcogenide (TMDC) material family and are direct band gap semiconductors. The optical band gap of monolayer MoS_2 and WS_2 is ∼1.9 and 2.0 eV, respectively. Ternary $Mo_xW_{1-x}S_2$ enables tuning of excitonic transition energy dependent on the concentration x.

Atomic layer deposition (ALD) is used to deposit $MoWS_2$ in the whole composition range between pure MoS_2 and WS_2. The concentration x is determined by the frequency position of the A_{1g} Raman mode. The distribution of W and Mo atoms in the crystal lattice of $MoWS_2$ is studied by high resolution scanning transmission electron microscopy. Additional annealing is performed to improve structural and optical properties. Photoluminescence spectroscopy measurements show concentration dependent spectral position of A and B excitonic emission.

DS 27.4 Fri 10:15 H36

Epitaxial growth of post transition metal chalcogenides: From standard approaches to new capabilities — •Eugenio Zallo[1,2], Michele Bissolo[1], Marco Dembecki[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter-Schottky-Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748, Garching, Germany — [2]Paul-Drude-Institut für Festkoerperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117, Berlin, Germany

Van der Waals (vdW) materials grown epitaxially are an urgent challenge for the development of scalable and high-crystalline-quality semiconductor films that can be exploited for novel device technologies. 2D materials "beyond graphene" have sparked immense interest in recent years, due to their excellent physical properties. Among them, post transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are vdW semiconductor materials with extraordinary photoresponsivity, a quasi-direct gap with a Mexican hat valence band and promising thermoelectric properties but they suffer from fast layer oxidation. In this presentation, the molecular beam epitaxy (MBE) growth of large-area PTMC is demonstrated on 3D and 2D bonded substrates by means of encapsulation strategies and careful microscopic and spectroscopic characterizations supported by density functional theory calculations. In order to study the pristine information of air sensitive materials, we present a cutting edge UHV cluster tool for the synthesis of ultrapure 2D-PTMCs and their heterostructures. The potential directions will be described.

DS 27.5 Fri 10:30 H36

Fabrication of Dielectric Mirrors and Microcavity Configurations for Light-Matter Coupling with Transition-Metal Dichalcogenides Heterostructures — •Chirag Palekar[1], Manan Shah[2], Fynn Kunze[2], Peter Klar[2], Stephan Reitzenstein[1], and Arash Rahimi-Iman[2] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623, Germany. — [2]I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany

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15 min. break

DS 27.6 Fri 11:00 H36

Selective area growth of MoS_2 via CVD on patterned GaN-AlO_x substrates — •Simon Wörle, Theresa Grünleitner, Alex Henning, and Ian Sharp — Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

Two-dimensional (2D) transition metal dichalcogenides have attracted considerable attention due to their unique optoelectronic properties. For the application of 2D materials in semiconductor devices, the controlled and scalable synthesis of high-quality 2D materials is critical.

Here, we demonstrate the selective area growth of MoS_2 by chemical vapor deposition (CVD) on GaN substrates that were patterned with ultrathin aluminum oxide coatings created by low-temperature atomic layer deposition. Optical and scanning electron microscopy images show that mono- and few-layer MoS_2 flakes preferentially nucleate and grow directly on the (uncoated) GaN. Atomic force microscopy and Raman measurements further reveal the formation of triangular and star-like shaped multilayer MoS_2 crystals at the interfaces between GaN and AlO_x. Moreover, the observed fixed orientation of the triangular MoS_2 flakes with respect to the GaN substrate lattice indicates van der Waals epitaxy. By altering the CVD growth conditions, the density of deposited MoS_2 flakes can be tuned, resulting in the growth of either isolated MoS_2 nanosheets or continuous films, in the latter of which the individual flakes have coalesced.

The presented results mark an important step towards integrated MoS_2 based heterostructures for semiconductor device applications.

DS 27.7 Fri 11:15 H36

Patterned growth of transition metal dichalcogenides monolayers and multilayers for electronic and optoelectronic device application — •Seung Heon Han[1], Ziyang Gan[1], Emad Najafidehaghani[1], Fatemeh Abtahi[2], Christof Neumann[1], Julian Picker[1], Tobias Vogel[2], Uwe Hübner[3], Falk Eilenberger[2], Antony George[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany

We present a simple, large area, cost effective soft lithographic method for growth of high-quality two-dimensional transition metal dichalcogenides (TMDs). Initially, a liquid precursor (Na2MoO4 in aqueous solution) is patterned on the growth substrate using micro-molding in capillaries (MIMIC) technique. Subsequently, a chemical vapor deposition (CVD) step is employed to convert the precursor patterns to monolayer, few layers, or bulk TMDs, depending on the precursor concentration. The grown patterns were characterized using optical microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy, and photoluminescence spectroscopy to reveal their morphological, chemical, and optical characteristics. The applicability of the grown patterned TMDs were tested for application such as field effect transistors, photodetectors, and memtransistor devices.

DS 27.8 Fri 11:30 H36

Conductive 2D MOFs in van-der-Waals heterostructures — •Jonas Pöhls[1], Zhiyong Wang[2], Renhao Dong[2], and Thomas Weitz[1] — [1]I. Physical Institute University of Göttingen, Göttingen, Germany — [2]Technical University of Dresden, Dresden, Germany

In conventional three-dimentional (3D) Metal-Organic Frameworks (MOFs) the electric conductivity is limited by the large separation of the metal centers by the organic ligands. Recent advantages in the synthesis of layered two-dimensional conjugated MOFs (2D c-MOFs) lead to a large improvement of the electronic properties, these materials allow a charge transfer along both interlayer (π-π-stacking) and intralayer (basal plane) directions [1]. In order to elucidate the underlying charge transport mechanisms in the 2D c-MOFs, we perform electronic characterizations of the films implemented in field-effect transistors under varying conditions. In addition to the improved properties of the 2D c-MOFs themselves, their 2D nature make them also a promising candidate for the fabrication of van-der-Waals heterostructures with other 2D materials like graphene, which could give access to a variety of interaction-driven effects. We present first results on the charge transport of 2D c-MOFs down to the size of single crystals as well as implemented in van-der-Waals heterostructures.

[1] Z. Wang et al. "Interfacial Synthesis of Layer-Oriented 2D Conjugated Metal*Organic Framework Films toward Directional Charge Transport", J. Am. Chem. Soc. (2021)

DS 27.9 Fri 11:45 H36

Controlled Encapsulation of Monolayer MoS2 with Ultrathin Aluminium Oxide for Tunnel Contacts — •Sergej Levashov, Chenjiang Qian, Theresa Grünleitner, Jon J. Finley, Alex Henning, and Ian D. Sharp — Walter Shottky Institut, TUM, München, Deutschland

Two-dimensional (2D) semiconductors have unique optoelectronic properties that provide the opportunity to overcome current scaling and performance limits of semiconductor devices. To harness the full of potential of 2D materials, requires their seamless integration with bulk materials. In particular, contacting mono- and few-layer 2D semiconductors with metals is challenging since the deposition process may introduce defects impeding interfacial charge transport. Here we use low-temperature atomic layer deposition to encapsulate monolayer MoS_2 with a van der Waals bonded and ultrathin aluminium oxide (AlO_x) layer. The 18 Å thin AlO_x coating introduces additional charge carriers ($\sim 5 \cdot 10^{12}$ cm^{-2}), while it also protects monolayer MoS_2 from defect creation during metallization. Microscratching of the AlO_x adlayer by contact mode atomic force microscopy and subsequent spectroscopic analysis demonstrate the reversibility of the charge transfer doping effect, indicating weak interaction. Importantly, current voltage measurements yielded a two-fold reduction in the contact resistance for MoS_2 field-effect transistors contacted with AlO_x interlayer. Overall, this work demonstrates the beneficial effect of the AlO_x adlayer for improving 2D device contacts and provides a scalable route to the damage-free integration of 2D semiconductors.