Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls H1, H3, and H5; Poster P)

Topical Talks

DS 5.1	Tue	13:30–14:00	H3	**Single crystal diamond grown by CVD: state of the art, current challenges and applications** — •Jean-Charles Arnault, Samuel Saada, Victor Ralchenko
DS 5.2	Tue	14:00–14:30	H3	**Tuning Semiconductor Mode-Locked Laser Frequency Combs by Gain and Cavity Design** — Stefan Meinecke, •Kathy Lüdge
DS 5.3	Tue	14:30–15:00	H3	**Monolayer-thick GaN/AlN heterostructures for UVB & UVC ranges: technology, design and properties** — Valentin Jmerik, Alexey Toropov, Valery Davydov, •Sergey Ivanov
DS 5.4	Tue	15:15–15:45	H3	**Optical and vibrational properties of layered 2D materials** — •Janina Maultzsch
DS 5.5	Tue	15:45–16:15	H3	**Organic/inorganic low dimensional material systems: Fundamental aspects and device applications** — •Emil List-Kratochvil
DS 6.1	Thu	13:30–14:00	H1	**Exceptional Topology of Non-Hermitian Systems: from Theoretical Foundations to Novel Quantum Sensors** — •Jan Carl Budich
DS 6.2	Thu	14:00–14:30	H1	**In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices** — •Peter Schüffelgen
DS 6.3	Thu	14:30–15:00	H1	**Atomic monolayers as two-dimensional topological insulators** — •Ralph Claessen
DS 6.4	Thu	15:15–15:45	H1	**Topological Insulator Lasers** — •Mordechai Segev
DS 6.5	Thu	15:45–16:15	H1	**TBA** — •Morais Smith

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Attosecond and coherent spins: New frontiers (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma, John Kay Dewhurst
SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber

SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium Physics of van der Waals 2D heterostructures (SYWH)

See SYWH for the full program of the symposium.

SYWH 1.1	Thu	13:30–14:00	Audimax 2	**Spin interactions in van der Waals topological materials and magnets** — •Saroj Dash
SYWH 1.2	Thu	14:00–14:30	Audimax 2	**Exciton optics, dynamics and transport in atomically thin materials** — •Ermin Malic, Samuel Brem, Raul Perea-Causin, Daniel Erkensten, Roberto Rosati
SYWH 1.3	Thu	14:30–15:00	Audimax 2	**Correlated Electrons in van der Waals Superlattices: Control and Understanding** — •Tim Wehling
SYWH 1.4	Thu	15:15–15:45	Audimax 2	**Exciton manipulation and transport in 2D semiconductor heterostructures** — •Andras Kis
SYWH 1.5	Thu	15:45–16:15	Audimax 2	**Chern Insulators, van Hove singularities and Topological Flatbands in Magic-angle Twisted Bilayer Graphene*** — •Eva Andrei, Shuang Wu, Zhenyuan Zhang

Sessions

DS 1.1–1.4	Mon	10:00–11:00	H3	**Thin Film Properties**
DS 2.1–2.7	Mon	11:15–13:00	H3	**2D materials and their heterostructures (joint session DS/HL/CPP)**
DS 3.1–3.9	Mon	13:30–16:15	H4	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS)**
DS 4.1–4.27	Tue	10:00–13:00	P	**Poster**
DS 5.1–5.5	Tue	13:30–16:15	H3	**Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)**
DS 6.1–6.5	Thu	13:30–16:15	H1	**Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)**
DS 7.1–7.4	Thu	15:15–16:15	H5	**Thin Oxides and Organic Thin Films (joint session DS/CPP)**
DS 8	Thu	18:00–19:00	MVDS	**Annual General Meeting of the Thin Films Division**
DS 9.1–9.4	Fri	10:00–11:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)**
DS 10.1–10.7	Fri	11:15–13:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)**
DS 11.1–11.5	Fri	13:30–14:45	H4	**2D semiconductors and van der Waals heterostructures II (joint session HL/DS)**

Annual General Meeting of the Thin Films Division

Donnerstag 18:00–19:00 MVDS

- Bericht
- Wahl
- Verschiedenes

DS 1: Thin Film Properties

Time: Monday 10:00–11:00 Location: H3

DS 1.1 Mon 10:00 H3

Ultra-thin lithium fluoride on Ag(100): growth and morphology — •Vladyslav Romankov and Jan Dreiser — Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Thin films of lithium fluoride (LiF) are of high interest for spintronic applications [1], and they can be potentially used as decoupling layers for single-molecule magnets [2] and other molecules. In the present work we show that two strikingly different morphologies of LiF/Ag(100) can be achieved by keeping the Ag substrate at two different temperatures during the deposition of LiF.

Polarized X-ray absorption spectroscopy, scanning tunneling microscopy and low energy electron diffraction reveal that LiF grows epitaxially, preferring a vertical growth over the layer-by-layer growth. At room temperature LiF forms anisotropic strained dendrites with branches parallel to the [011] and [0$\bar{1}$1] directions of the substrate. Conversely, at a substrate temperature of 500 K LiF assembles into more relaxed square islands displaying a Moiré pattern. The strong qualitative difference between the two morphologies makes LiF/Ag(100) an interesting model system to study the dependence of the growth kinetics on the temperature.

References: [1] A. J. Drew et al., Nature Materials, **8**, 109, (2009); [2] C. Wäckerlin et al., Advanced Materials, **28**, 5142, (2016).

DS 1.2 Mon 10:15 H3

Stacking fault fold and step junctions as nucleation sites of threading dislocations in III-nitride films — •Georgios Dimitrakopulos[1], Isaak Vasileiadis[1], Joanna Moneta[2], Polyxeni Chatzopoulou[1], Philomela Komninou[1], and Julita Smalc-Koziorowska[2] — [1]Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece — [2]Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

III-nitride semiconductor heterostructures have been employed with great success in optoelectronic and electronic devices despite the high densities of threading dislocations (TDs) that they contain. In order to unlock the full potential of these materials, it is imperative to diminish the TD nucleation sites. We present a mechanism of TD nucleation taking place at folds and steps of basal stacking faults (BSFs), particularly intrinsic I1 BSFs, that are frequent in (0001) epilayers due to their low self-energy. In-depth analysis by transmission electron microscopy (TEM) revealed that TD introduction is geometrically necessary at nodes of Shockley-like partial dislocations (PDs) at such BSFs. These PDs have the same Burgers vectors as normal Shockley PDs but exist only at junctions of the two variants of the BSF stacking sequence. In I1 BSF overlaps, the introduction of Frank-Shockley PDs is avoided, thus eliminating the elastic strain along the growth direction. Overlapped BSFs were observed to form hexagonal closed domains in which the coexistence of PD segments makes TD nucleation energetically favorable.

DS 1.3 Mon 10:30 H3

Cellulose nanofibrils as sustainable template material for thin silver nanowire electrodes fabricated via spray deposition — •Marie Betker[1,2], Constantin Harder[1,3], Elisabeth Erbes[1,4], Matthias Schwartzkopf[1], Andrei Chumakov[1], Daniel L. Söderberg[2], and Stephan V. Roth[1,2] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 8, 10044 Stockholm, Sweden — [3]Physik-Department E13, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [4]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Goettingen, Germany

Cellulose nanofibrils (CNFs) are wood-based, lightweight, and flexible, making them suitable for the fabrication of sustainable composite materials. With spray deposition the preparation of thin, homogenous CNF films of large scale and with an low roughness as well as their functionalization with e.g. nanoparticles is possible. We use CNF as a sustainable template material for the fabrication of two different types of thin silver nanowire (AgNW) electrodes via spray deposition: (I) A layered structure of a AgNW-network on top of a thin CNF layer and (II) a thin layer consisting of a mixture of CNF and AgNW. We compare the structural and electrical properties of both types using SEM, AFM, grazing incidence small angle X-ray scattering (GISAXS), and four-point measurements. The results demonstrate that type (II) is more conductive, leading to the conclusion that CNF has beneficial templating effects on the electronic properties of the AgNW network.

DS 1.4 Mon 10:45 H3

Epitaxial growth of $(Cr_{1-x}Fe_x)_2AlC$ MAX Phase thin films by pulsed laser deposition — •Hanna Pazniak[1], Marc Stevens[1], Martin Dahlqvist[2], Benjamin Zingsem[1,3], Johanna Rosen[2], Michael Farle[1,4], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [2]Thin Film Physics Division, Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany — [4]Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Russian Federation

MAX phase epitaxial thin films attract increasing attention with respect to high-temperature applications [1]. The partial substitution of M atoms in their nanolaminated structure is a promising way to tailor magnetic properties. In this study, we synthesized $(Cr_{1-x}Fe_x)_2AlC$ ($0<x<0.2$) epitaxial thin films by Pulsed Laser Deposition on MgO(111) and Al_2O_3(0001) at 600°C using pure elemental targets. By combining structural characterization and density functional theory, we explored the phase composition of synthesized $(Cr_{1-x}Fe_x)_2AlC$ solid solutions, finding a Fe solubility limit of 4 at.%. Excess Fe leads to the formation of the $(Cr,Fe)_5Al_8$ intermetallic secondary phase.

[1] M. Stevens, H. Pazniak, et al., MRL 9, 343 (2021).

Funding by the DFG within CRC/TRR 270, project B02 (Project-ID 405553726) is acknowledged.

DS 2: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00 Location: H3

DS 2.1 Mon 11:15 H3

Tunable phases of Moire excitons in van der Waals heterostructures — •Samuel Brem[1], Christopher Linderälv[2], Paul Erhart[2], and Ermin Malic[1,2] — [1]Philipps University, Marburg, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

Two monolayers of Transition Metal Dichalogenides can be vertically stacked to form a type-II heterostructure, hosting spatially indirect interlayer excitons. Recent studies have shown that moire superlattices can be created by stacking monolayers with a finite twist-angle, giving rise to a tunable modification of exciton features in optical spectra. The moire patterns lead to a spatially varying band gap and consequently, excitons experience a periodic potential modifying their transport properties.

We have combined first-principles calculations with the excitonic density matrix formalism to develop an exciton model for small-angle twisted MoSe2/WSe2 heterostructures. Based on a microscopic approach, we calculate the band structure and wave functions of intra- and interlayer excitons within a twist-tunable moire lattice as well as the resulting optical response. For a range of small twist-angles, we predict completely flat exciton bands corresponding to moire trapped, localized quantum emitters. However, we reveal that this moire exciton phase quickly changes with increasing twist-angle, and at 3°, there are only delocalized excitons. We find the emergence of multiple moire exciton peaks in the absorption, whose spectral shifts with varying twist-angle are characteristic for the trapped or delocalized phase.

DS 2.2 Mon 11:30 H3

Electrical control of spin-orbit coupling-induced spin precession and spin-to-charge conversion in graphene proximitized by WSe2 — •Franz Herling[1], Josep Ingla-Aynes[1], C. K. Safeer[1], Nerea Ontoso[1], Jaroslav Fabian[2], Luis E. Hueso[1,3], and Felix Casanova[1,3] — [1]CIC nanoGUNE BRTA, Spain — [2]University of Regensburg, Germany — [3]IKERBASQUE, Basque Foundation for Science, Spain

When combined with WSe2, a large spin-orbit coupling gets imprinted by proximity effect into graphene. Here, we use this effect to achieve the strong SOC regime in bilayer graphene. Together with the long, gate tunable spin diffusion, this provides unique control knobs to manipulate coherent spin precession in the absence of an external magnetic field. Remarkably, we observe in these devices that the sign of the precessing spin polarization can be tuned electrically by a back gate voltage and by a drift current. This realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal of spintronics, could be a cornerstone for the implementation of energy efficient spin-based logic.

In accordance with the large proximity-induced SOC, we also observe spin Hall effect in similar heterostructures with an unprecedented spin-to-charge conversion length of up to 41 nm. Such highly efficient conversion up to room temperature will play a crucial role for the future integration of spintronic devices into existing electronic infrastructure.

DS 2.3 Mon 11:45 H3

Gate-Switchable Arrays of Quantum Light Emitters in Contacted Monolayer MoS_2 van der Waals Heterodevices — •Alexander Hötger[1,2], Julian Klein[1,2,3,4], Katja Barthelmi[1,3], Lukas Sigl[1,2], Samuel Gyger[5], Takashi Taniguchi[6], Kenji Watanabe[6], Val Zwiller[5], Klaus D. Jöns[5], Ursula Wurstbauer[2,7], Jonathan Finley[1,2,3], and Alexander Holleitner[1,2,3] — [1]Walter Schottky Institut, TU Munich — [2]Exzellenzcluster e-conversion — [3]Munich Center for Quantum Science and Technology — [4]Massachusetts Institute of Technology, Cambridge — [5]KTH Royal Institute of Technology, Dept. of Applied Physics — [6]National Institute for Materials Science, Tsukuba — [7]Institute of Physics, Westfälische Wilhelms-Universität Münster

Controlling single-photon emission on a few nanometers plays an important role for the scalability of future quantum photonic circuits. Moreover, it is highly relevant to facilitate a gate-switchable emission for quantum information schemes. By irradiating MoS_2 with helium ions, we generate single-photon sources at ∼1.75 eV with a lateral position accuracy of only a few nanometers. [1] Second-order correlation measurements unambiguously proof the nature of single-photon emission. Charge doping of the monolayer MoS_2 can be used for switching the quantum emission on and off. [2] This deterministic control of light emission in spatial and temporal means paves the way for new integrated quantum photonic technologies.

[1] J. Klein, L. Sigl et al., ACS Photonics 8, 2 (2021).
[2] A. Hötger et al., Nano Lett. 21, 2 (2021).

DS 2.4 Mon 12:00 H3

Tunnelling transport in bilayer graphene nanostructures with quantum dots — •Angelika Knothe[1], Vladimir Fal'ko[1], and Leonid Glazman[2] — [1]National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, e.g., transistors or qubits. In gapped bilayer graphene (BLG), one can confine charge carriers electrostatically, inducing smooth confinement potentials while allowing gate-defined control of the confined structure. I will discuss charge transport in BLG nanostructures with electrostatically confined quantum dots. We investigate both theoretically and in collaboration with experiments how the BLG dots' highly degenerate single- and two-electron spin and valley multiplets, which depend on, e.g., the displacement field and the electron-electron interactions, manifest in tunnelling transport. This way, we shed light on BLG material parameters while opening the field for using the dots' rich spin and valley multiplets for quantum information.

1) Theory of tunneling spectra for a few-electron bilayer graphene quantum dot, A. Knothe, L. Glazman, V. Fal'ko, arXiv:2104.03399 2) Probing two-electron multiplets in bilayer graphene quantum dots, S. Möller, L. Banszerus, A. Knothe, L. Glazman, V. Fal'ko, C. Stampfer, et. al, arXiv:2106.08405 3) Quartet states in two-electron quantum dots in bilayer graphene, A. Knothe, V. Fal'ko, PRB 101, 235423 (2020)

DS 2.5 Mon 12:15 H3

Unconventional Superconductivity in Magic-Angle Twisted Trilayer Graphene — •Ammon Fischer — Institute for Theory of Statistical Physics, RWTH Aachen University

Magic-angle twisted trilayer graphene (MATTG) recently emerged as a highly tunable platform for studying correlated phases of matter, such as correlated insulators and superconductivity. Superconductivity occurs in a range of doping levels that is bounded by van Hove singularities which stimulates the debate of the origin and nature of superconductivity in this material. In this work, we discuss the role of spin-fluctuations arising from atomic-scale correlations in MATTG for the superconducting state. We show that in a phase diagram as function of doping (ν) and temperature, nematic superconducting regions are surrounded by ferromagnetic states and that a superconducting dome with $T_c \approx 2$ K appears between the integer fillings $\nu = -2$ and $\nu = -3$. Applying a perpendicular electric field enhances superconductivity on the electron-doped side which we relate to changes in the spin-fluctuation spectrum. We show that the nematic unconventional superconductivity leads to pronounced signatures in the local density of states detectable by scanning tunneling spectroscopy measurements.

DS 2.6 Mon 12:30 H3

Twist angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide heterostructures — •Thomas Naimer[1], Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

We investigate proximity-induced spin-orbit coupling (SOC) in graphene on the four transition-metal dichalcogenides (TMDCs) MoS_2, WS_2, $MoSe_2$ and WSe_2 from first principles. By using different supercells of graphene/TMDC heterostructures we provide systematic insight on the effect of twist angles on the low energy Dirac spectrum. We find that the exact position of the Dirac cone within the TMDC band gap depends linearly on the biaxial strain applied to the graphene. From this relation we extrapolate the zero-strain band offset and correct the band offsets of all calculations by employing a transverse electric field across the heterostructure. The corrected results reveal massive twist angle tunability of both the magnitude and flavor of proximity induced SOC: We observe a peak in SOC at approximately 19° twist angle and vanishing SOC at 30°. This work was supported by ENB "Topologische Isolatoren" and SFB 1277.

DS 2.7 Mon 12:45 H3

Predicting the adsorption of alkali metals on 2D materials — Maofeng Dou and •Maria Fyta — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The adsorption of alkali metal atoms on two-dimensional transition metal dichalcogenides (2D TMDCs) is investigated using quantum-mechanical calculations. Specifically, we evaluate the adsorption characteristics of Li on 2D TMDCs through the respective adsorption energies. We decompose these energies into separate components in order to fundamentally understand the adsorption process. The adsorption energies of lithium on 2D TMDCs were found to strongly and linearly correlate with the energy of the lowest unoccupied states of the materials. Accordingly, we propose and demonstrate the use of this energy as a descriptor for predicting adsorption energies. We further proceed with additional 2D TMDCs and adsorbed alkali atoms in order to generate a database that allows us to learn and make predictions. Our results strongly support the use of the energy of the lowest unoccupied states as a novel efficient descriptor for a data-driven design of materials with pre-selected properties and functions for target applications.

DS 3: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS)

Time: Monday 13:30–16:15 Location: H4

Invited Talk DS 3.1 Mon 13:30 H4

The role of chalcogen vacancies for atomic defect emission in MoS_2 — Elmar Mitterreiter[1], Bruno Schuler[2], Daniel Hernangómez-Pérez[3], Julian Klein[4], Jonathan Finley[1], Sivan Refaely-Abramson[3], Alexander Holleitner[1], Alexander Weber-Bargioni[5], and •Christoph Kastl[1] — [1]Walter Schottky Institute, TU Munich — [2]nanotech@surfaces Laboratory, Empa — [3]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science — [4]Massachusetts Institute of Technology — [5]Molecular Foundry, Lawrence Berkeley National Laboratory

The microscopic understanding of defect-related modifications in 2D materials requires correlation between atomic structure and resulting macroscopic electronic, optical or excitonic properties. Combing controlled defect engineering with optical spectroscopy as well as atomic imaging and ab-initio theory, we identify the optical signature of pristine chalcogen vacancies in single layer MoS_2. [1] Vacancies introduce a narrow optical emission, markedly different from previously observed broad luminescence bands. Comparing annealed vs. He-ion treated MoS_2, we establish that the recently discovered single-photon emitters in He-ion irradiated MoS_2 originate from chalcogen vacancies. Using focused ion beam irradiation, the latter can be created site-selectively [2] with a spatial precision better than 10 nm [3], which is important for a prospective integration of defect-based single photon emitters into quantum photonic circuits. [1] E. Mitterreiter et al., Nat. Commun. 12, 3822 (2021). [2] J. Klein et al. ACS Photonics 8, 669-677 (2021). [3] E. Mitterreiter et al., Nano Lett. 20, 4437 (2020).

DS 3.2 Mon 14:00 H4

Coherent light emission of exciton-polaritons in an atomically thin crystal at room temperature — •Hangyong Shan[1], Lukas Lackner[1], Bo Han[1], Evgeny Sedov[2], Falk Eilenberger[4], Sebastian Klembt[3], Sven Höfling[3], Alexey V. Kavokin[2], Christian Schneider[1], and Carlos Anton-Solanas[1] — [1]Institute of Physics, Carl von Ossietzky University, 26129 Oldenburg, Germany. — [2]School of Science, Westlake University, 310024 Hangzhou, People's Republic of China. — [3]Technische Physik, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany. — [4]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University, 07745 Jena, Germany.

We experimentally study the coherence of exciton-polaritons in a Fabry-Perot microcavity loaded with an atomically thin WSe2 layer. Via Michelson interferometry, we capture clear evidence of increased spatial and temporal coherence of the emitted light from the spatially confined system ground-state. The coherence build-up is accompanied by a threshold-like behaviour of the emitted light intensity, which is a fingerprint of a polariton condensation effect. Valley-physics is manifested in the presence of an external magnetic field, which allows us to manipulate K and K* polaritons via the Valley-Zeeman-effect. Our findings are of high application relevance, as they confirm the possibility to use atomically thin crystals as simple and versatile components of coherent light-sources, and in valleytronic applications at room temperature.

DS 3.3 Mon 14:15 H4

Bosonic condensation of exciton-polaritons in an atomically thin crystal — •Carlos Anton-Solanas[1,2], Maximilian Waldherr[1], Martin Klaas[1], Holger Suchomel[1], Tristan H. Harder[1], Hui Cai[3], Evgeny Sedov[4], Sebastian Klembt[1], Alexey V. Kavokin[4], Sefaattin Tongay[5], Kenji Watanabe[6], Takashi Taniguchi[6], Sven Hoefling[1], and Christian Schneider[2] — [1]Univ. Wuerzburg, Germany — [2]Univ. Oldenburg, Germany — [3]Univ. California, USA — [4]Westlake Univ., China — [5]Arizona State Univ., USA — [6]Nat. Institute for Materials Science, Japan

Semiconducting monolayer crystals have emerged as a new platform for studies of tightly bound excitons and many-body excitations in ultimately thin materials. Their giant dipole coupling to optical fields makes them very appealing for (nano-) photonic devices, and for fundamental investigations in the framework of cavity quantum electrodynamics.

Our experiments demonstrate the strong light-matter coupling and, for the first time, the bosonic condensation of exciton-polaritons in an atomically thin layer of $MoSe_2$ coupled to a hybrid micro-cavity [1].

We demonstrate the emergence of long-range first-order spatial coherence, via interferometric $g^{(1)}(\tau)$ measures, and we have investigated the Zeeman splitting effects of condensed polaritons under strong magnetic fields.

[1] Anton-Solanas, C., Waldherr, M., Klaas, M. et al. Bosonic condensation of exciton polaritons in an atomically thin crystal. Nat. Mater. (2021).

DS 3.4 Mon 14:30 H4

Hybridization between monolayer transition-metal dichalcogenides and conjugated molecular adsorbants — •Jannis Krumland[1] and Caterina Cocchi[1,2] — [1]Humboldt-Universität zu Berlin — [2]Carl von Ossietzky Universität Oldenburg

We present a first-principles study on electronic hybridization in inorganic-oraganic interfaces composed of monolayer transition-metal dichalcogenides (TMDCs; molybdenum and tungsten disulfide and diselenide) and exemplary carbon-conjugated molecules such as pyrene and perylene. By means of band-structure unfolding techniques applied to hybrid density-functional theory calculations including spin-orbit coupling, we achieve an intuitive and clear description of electronic interaction between the inorganic and organic components of the heterostructures. From atom-projected band structures, we are able to rationalize the strong mixing between the valence states of the TMDC and the molecular orbitals. We additionally clarify why the highest occupied orbital couples with the TMDC bands only very weakly, regardless of the composition of the interface. The proposed analysis based on band structure unfolding lends itself for computationally efficient and yet reliable predictions of electronic interactions in more complex hybrid interfaces including larger molecules harvesting visible radiation.

DS 3.5 Mon 14:45 H4

Tunable Polymer/Air Bragg Optical Microcavity Configurations for Light-Matter Coupling with Transition-Metal Dichalcogenides and their Heterostructures — •Chirag Palekar[1,2], Stephan Reitzenstein[1], and Arash Rahimi-Iman[2] — [1]Present address: Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

Light-matter interactions (LMI) in semiconducting materials is being studied extensively with the help of optical microcavities. Specifically, tunable microcavities provide a versatile platform to control the LMI between the material excitation and cavity photons. Here, we explore a new resonator approach which can be employed to achieve microscopic photonic Fabry-Pérot (FP) cavities with mechanically- tunable resonator modes and polymer/air Bragg mirrors [1], directly on a chip or device substrate in combination with active materials. Moreover, our simulations based on the transfer matrix method show, compression-induced mode control of the air-Bragg cavities enables tuning between the weak and strong coupling regime. Using this unique cavity configurations, LMI experiments with 2D semiconductors such as transitionmetal dichalcogenides (TMDC) are very attractive. Additionally, incorporation of TMDC heterostructures in FP cavities will provide a platform to understand the new regimes of Dicke superradiance as well as Bose-Einstein condensation of Moiré exciton-polaritons. Ref.: [1] Phys. Status Solidi RRL 2021, 15, 2100182

15 min. break

DS 3.6 Mon 15:15 H4

Phonon-assisted exciton dissociation in transition metal dichalcogenides — •Raul Perea-Causin[1], Samuel Brem[1], and Ermin Malic[1,2] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Philipps-Universität, Marburg, Germany

Monolayers of transition metal dichalcogenides (TMDs) have been established in the last years as promising materials for novel optoelectronic devices. However, the performance of such devices is often limited by the dissociation of tightly bound excitons into free electrons and holes. While previous studies have investigated tunneling at large electric fields, we focus in this work on phonon-assisted exciton dissociation that is expected to be the dominant mechanism at small fields.

We present a microscopic model based on the density matrix formalism providing access to time- and momentum-resolved exciton dynamics including phonon-assisted dissociation [1]. We track the pathway of excitons from optical excitation via thermalization to dissociation, identifying the main transitions and dissociation channels. Furthermore, we find intrinsic limits for the quantum efficiency and response time of a TMD-based photodetector and investigate their tunability with externally accessible knobs, such as excitation energy, substrate screening, temperature and strain.

Our work provides microscopic insights in fundamental mechanisms behind exciton dissociation and can serve as a guide for the optimization of TMD-based optoelectronic devices.

[1] R. Perea-Causin et al., Nanoscale 13, 1884 (2021)

DS 3.7 Mon 15:30 H4

Lattice Configurations of Self-Assembled Folded Graphene — •Lina Bockhorn, Johannes C. Rode, Lucas Gnörich, Pengfei Zuo, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The stacking- and folding angle of 2D materials to 3D structures has emerged as an important, novel tuning parameter for the tailoring of optical, mechanical, electronic and magnetic properties. Therefore, it is highly desirable to gather insight into the mechanical formation of these structures on the nano-scale.

Here, we focus on the evolution of self-assembled folded graphene generated via atomic force microscopy technique, which could give a deep insight into its underlying growth energy [1, 2, 3]. The self-assembly process involves the folding-over of the graphene layer and the subsequent growth of a twisted graphene bilayer. We conclude, that these self-assembled structures move not only forward during the growth process but also appear to rotate and lock in at specific commensurate twist angles.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).

DS 3.8 Mon 15:45 H4

All-optical polarization and amplitude modulation of second harmonic generation in atomically thin semiconductors — •Sebastian Klimmer — Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany

Nonlinear optics is of paramount importance in several fields of science and technology. This is particularly true in the case of second harmonic generation (SHG), which is commonly used for frequency conversion, self-referencing of frequency combs, crystal characterization, sensing, and ultra-short pulse characterization. Large efforts have been devoted in the last years to realizing electrical and all-optical modulation of SHG in atomically thin materials, which are easy to integrate on photonic platforms and thus ideal for novel nano-photonic devices. Here, we propose a new approach to broadband all-optical modulation of SHG in 2D materials. Our concept is based only on symmetry considerations and thus is applicable to any material of the D3h symmetry group and with deep sub-wavelength thickness, such as all monolayer transition metal dichalcogenides. With this approach we demonstrate a 90° rotation of the polarization of the emitted SH on a time-scale limited only by the fundamental pulse duration. In addition, this ultrafast polarization switch can be immediately applied to realize all-optical SH amplitude modulation with depth of 100 %. Our results outperform any previous work on all-optical SHG modulation [1,2] in terms of modulation speed, modulation depth and SHG bandwidth.

[1] Taghinejad M. *et al.*, Small **16**, 1906347 (2020)
[2] Cheng Y. *et al.*, Nano Lett. **20**, 11 (2020) 8053-8058

DS 3.9 Mon 16:00 H4

Microscopic Theory of Exciton-Exciton Annihilation in Two-Dimensional Semiconductors — •Alexander Steinhoff, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Auger-like exciton-exciton annihilation (EEA) is considered the key fundamental limitation to quantum yield in devices based on excitons in two-dimensional (2d) materials. Since it is challenging to experimentally disentangle EEA from competing processes, guidance of a quantitative theory is highly desirable. The very nature of EEA requires a material-realistic description that is not available to date.

We present a many-body theory of EEA based on first-principle band structures and Coulomb interaction matrix elements that goes beyond an effective bosonic picture. Applying our theory to monolayer MoS_2 encapsulated in hexagonal BN, we obtain an EEA coefficient in the order of 10^{-3} cm^2s^{-1} at room temperature, suggesting that carrier losses are often dominated by other processes, such as defect-assisted scattering.

Our studies open a perspective to quantify the efficiency of intrinsic EEA processes in various 2d materials in the focus of modern materials research.

DS 4: Poster

Time: Tuesday 10:00–13:00 Location: P

DS 4.1 Tue 10:00 P

Two-color time-resolved Kerr rotation measurements of twisted MoS_2/WS_2 heterostructures — •Michael Kempf[1], Alina Schubert[1], Annika Bergmann[1], Mustafa Hemeid[1], Antony George[2], Andrey Turchanin[2], Rico Schwartz[1], and Tobias Korn[1] — [1]University of Rostock, Rostock, Germany — [2]University of Jena, Jena, Germany

Transition metal dichalcogenides (TMDC) have revealed many intriguing properties in recent years. For valleytronics especially, the coupling of spin and valley degrees of freedom shows great promise. Using valley-selective optical selection rules, a coupled spin-valley polarization can easily be introduced in these systems. Keeping possible future applications in mind, the dynamics of this polarization, especially its lifetime, is of great importance. Yet in pristine monolayer TMDCs this is strongly limited due to ultrafast optical exciton recombination and electron-hole exchange interaction. By contrast, in TMDC heterostructures, ultrafast interlayer charge transfer may circumvent these limits on valley polarization lifetimes.

We use two-color time-resolved Kerr rotation measurements to study the spin-valley dynamics in disulfide-based TMDCs and their heterostructures. The independent tunability of our coupled laser systems allows to selectively pump and probe their excitonic transitions resonantly. We present low-temperature valley dynamics studies on TMDC monolayers and twisted MoS2-WS2 heterostructures fabricated by combining CVD-grown and exfoliated monolayers.

DS 4.2 Tue 10:00 P

Revealing in plane g factors in multilayer WSe2 via time-resolved Faraday experiments — •Simon Raiber, Dennis Falter, and Christian Schüller — Universtiät Regensburg

With the increasing investigation of two-dimensional heterostructures, the question arises how far the layer-intrinsic properties are imparted to multilayer van der Waals structures. While the effects of external magnetic fields on transition metal dicalcogenides monolayers have been studied intensively during the last years, the interaction of multiple layers remained largely disregarded.

We demonstrate a non-zero effective g factor for in plane magnetic fields in few-layer WSe2 making use of time-resolved Faraday rotation experiments. The found values commensurate to the established out of plane effective g factors. This indicates an isotropic effective in plane g factor for multilayer WSe2, which stands in contrast to monolayer samples. Up to now no standard theoretical approach can model an non-zero in plane g factor.

DS 4.3 Tue 10:00 P

Controlled moirè potentials of MoSe2/WSe2 heterostructures for time resolved kerr measurments — •Andreas Beer, Philipp Parzefall, Laura Zinkl, Anna Weindl, and Christian Schüller — Universität Regensburg

In heterostructures the twist angle serves as an degree of freedom to severly manipulate exciton dynamics.

We fabricate heterostructures with advanced twist angle control by staking CVD-grown triangulars of TMDCs.

To track the excitons dynamics on the femtosecond timescale we use

two color pump probe measurements.

DS 4.4 Tue 10:00 P

Strong coupling of Bloch Surface Waves and excitons in ZnO up to 430 K — •Sebastian Henn, Marius Grundmann, and Chris Sturm — 1Universität Leipzig, Faculty of Physics and Earth Sciences, Felix-Bloch institute for solid state physics, Linnéstr. 5, 04103 Leipzig, Germany

Exciton-polaritons are bosonic quasi-particles consisting of a cavity photon and an electron-hole pair, exhibiting interesting physical phenomena like Bose-Einstein condensation [1]. Of special interest are exciton-polaritons in semiconductors with large exciton binding energies, where the strong coupling is observable above room temperature [2]. We report here on the experimental observation of the strong coupling between ZnO excitons and Bloch Surface Waves (BSW) up to 430 K. The sample consists of a Bragg reflector and a thin ZnO top layer. This system holds several advantages compared to exciton-polaritons in conventional microcavities: high propagation lengths due to the low loss BSW with large in-plane wave vector, a reduced complexity of production and direct access to the mode-supporting surface layer. In combination with a stable operation at high temperatures, this is of interest for the development of integrated optics devices. By means of a prism coupler in reflection geometry the polariton dispersion was observed and analyzed. We determined the temperature dependent coupling strength, exciton energy and dielectric background.

[1] J. Klaers *et al.*, Nature **468**, 545-548 (2010)
[2] C. Sturm *et al.*, New J. Phys. **11**, 073044 (2009)

DS 4.5 Tue 10:00 P

Novel 2D surface alloys on Pt(111): electronic and structural properties — •Marta Przychodnia[1], Tomasz Grzela[1], Roland Wiesendanger[2], and Maciej Bazarnik[1,2] — [1]Institute of Physics, Poznan University of Technology, Poznan, Poland — [2]Department of Physics, Hamburg University, Hamburg, Germany

Lately, a new class of 2D magnetic films has been discovered, namely rare earth (RE) metals - transition metals (TM) surface alloys. Limiting the dimensionality of RE-TM alloys to 2D (so-called surface alloys) influences their properties in surprising ways. For example, a $GdAu_2$ and $GdAg_2$ surface alloys are ferromagnetic while in bulk they are antiferromagnetic. Small change of Au to Ag in this system raise the Curie temperature from 19°C to 85°C showing potential for tuneability.

Here, I will present the comparison study of Dy-Pt and Gd-Pt mono- and double-layers of surface alloys grown on Pt(111). Structural and electronic properties in atomic scale of both systems were investigated using scanning tunneling microscopy (STM) and spectroscopy (STS).

DS 4.6 Tue 10:00 P

Measuring Material-Specific Properties with Ultra-High Vacuum Atomic Force Microscopy — •Frederic Luis Condin, Jesús Sánchez Lacasa, and Baran Eren — Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel

The real-space imaging capabilities provided by scanning probe microscopy techniques have undoubtedly revolutionized the scientific study of surfaces and processes happening thereon. Whereas scanning tunneling microscopy is limited to conductive samples, atomic force microscopy can be used for any surface. A general problem of scanning probe microscopy is its lack of element specificity, i.e., it cannot be used for the identification of materials or adsorbed surface species without additional information or prior knowledge about the sample. We address this problem and present contributions towards the chemical identification of surface materials. To this end, we calculate Hamaker constants on different points of a sample from bias voltage and tip-sample distance dependent measurements of the frequency shift in amplitude and frequency modulation atomic force microscopy.

DS 4.7 Tue 10:00 P

Coordinated Development of Tubes and Optics: New possibilities for X-ray Analytics — •Jörg Wiesmann, Moritz Schlie, Jürgen Graf, Frank Hertlein, and Paul Radcliffe — Incoatec GmbH, Max-Planck-Strasse 2, 21502 Geesthacht

At Incoatec, we have a long history of offering solutions driven by the needs of the customers. As a specialist for multilayer optics we penetrated the crystallography market with our complete IμS Microfocus Solutions in 2006. Optics can only evolve their whole strength when the source is also matched to it. Due to this fact, we started in 2011 with the in-house development of X-ray sources. The aim was to offer the best combination of optics and sources for certain applications in small and macromolecular structure analysis. We were able to launch new solutions like the IμS3.0 and the IμS DIAMOND that offers a flux density of more than $5*10^{10}$ ph/s/mm^2 within a spot of less than 100μm. This high flux density is achieved with a low power air-cooled source that doesn't need maintenance during the typical life time of more than 6 years. We will summarize the key parameters for combining multilayer optics and microfocus tubes to achieve collimated or focused X-ray sources with high brilliance. The main part of the talk will explain the application-dependent design of our metal-ceramic tubes and how to match them with our multilayer optics. Applications include crystallography, nanotechnology and thin film research.

DS 4.8 Tue 10:00 P

Persistent response in ultra-strongly driven mechanical membrane resonators — •Fan Yang[1], Felicitas Hellbach[1], Felix Rochau[1], Wolfgang Belzig[1], Eva Weig[1,2], Gianluca Rastelli[3], and Elke Scheer[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Fakultät für Elektrotechnik und Informationstechnik, Technische Universität München, 80333 München, Germany — [3]INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy

We study experimentally and theoretically the phenomenon of *persistent response* in ultrastrongly driven membrane resonators. The term persistent response denotes the development of a vibrating state with nearly constant amplitude over an extreme wide frequency range of more than 50% of the eigenfrequency. This phenomenon is unusual and is key to avoid breakdown, since it imposes a self-limitation of the maximum amplitude. We reveal the underlying mechanism by directly imaging the vibrational state using advanced optical interferometry. We argue that this state is related to the nonlinear interaction between higher-order flexural modes and higher-order overtones of the driven mode. Finally, we propose a stability diagram for the different vibrational states that the membrane can adopt.

DS 4.9 Tue 10:00 P

Tunable frequency comb in flexural-mode-coupling regime in nonlinear mechanical membrane resonators — •Mengqi Fu, Fan Yang, and Elke Scheer — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Multimode coupling in mechanical systems has attracted broad interest in many realms of physics[1,2]. Recently, the research on the multimode coupling has been extended to strong nonlinear systems and novel phenomena have been observed caused by the strong nonlinearity of the coupled flexural modes[2]. Here, we demonstrate a novel tunable frequency comb generated by driving the mechanical system into the strongly nonlinear regime, i.e. the flexural-mode-coupling regime, by one-tone excitation. The studied system is based on a suspended SiN membrane ($\sim$ 500 nm thickness) with a quality factor of $\sim$ 19000. The frequency separation between neighboring sidebands of the frequency comb strongly depends on the damping factor, nonlinearity, vibration amplitude and the detuning frequency of the two coupled flexural modes. The frequency separation is tunable by varying the detuning frequency and the strength of the drive power. By systematically investigating the frequency response of the fluctuations close to the coupled flexural modes, we show that the observed frequency comb is generated when the "very states"[3] produced by the nonlinearity of the coupled flexural modes are crossed experimentally.

1. A. Ganesan et al., Phys. Rev. Lett. 118, 033903 (2017).
2. F. Yang et al., Phys. Rev. Lett. 127, 014304 (2021).
3. J.S. Huber et al., Phys. Rev. X, 10, 021066 (2020).

DS 4.10 Tue 10:00 P

Forming-free resistive switching in amorphous gallium oxide device — •Aman Baunthiyal[1], Jon-Olaf Krisponeit[1], Christian Habben[1], Alexander Karg[1], Martin Eickhoff[1], Sandra Pérez Domínguez[2], Manfred Radmacher[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Biophysics, University of Bremen, Germany

Currently, semiconductor based devices are reaching their limitations in terms of scalability and long time storage capability. To overcome this problem, inorganic and organic materials which show resistive switching (utilized in ReRAMs), magnetic switching (MRAMs), and phase change switching (PCRAMs) have been studied over the past 40 years. In ReRAMs, a repeatable switching between high resistive state (HRS) and low resistive state (LRS) can be observed when a voltage

sweep is applied across an active layer sandwiched between two metal electrodes.

In this study, the forming-free bipolar resistive switching was observed in a Al/GaO_x(76 nm)/Ru devices. The observed switching was proposed to be connected to the formation and rupture of conductive filaments constituted by oxygen vacancies in the GaO_x film. X-ray photoelelectron spectroscopy (XPS) analysis confirmed the high amount of oxygen vacancies in the GaO_x film. The LRS was found to be of ohmic nature, while the HRS followed Poole-Frenkel emission model. Due to their stable endurance cycle and long retention time with more than 10^3 order resistance ratio ,the devices can be regarded as promising prototypes for future non-volatile ReRAMs.

DS 4.11 Tue 10:00 P

Adsorption of fluids on hydrophobic surfaces under sub- and supercritical conditions — •Mike Moron, Göran Surmeier, Marc Moron, Jennifer Bolle, Susanne Dogan, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Adsorption at interfaces is crucial for many industrial applications, e. g. adsorption-based separation, regeneration of adsorbents in purification processes as well as for natural gas storage. In subcritical systems the adsorption layers of different fluids had been successfully described as molecular thin layers. The layer thickness diverges when the pressure reaches the condensation pressure of the corresponding fluid, meaning that the adsorption layer transforms into a macroscopic condensate. Supercritical adsorption, however, is far less understood on a molecular scale because of the complex requirements to the experimental environment, although the phenomenon is of outstanding importance for many applications. For example, the use of supercritical CO_2 is a gentle method to dry porous materials without damaging the frameworks. We investigated the pressure dependent adsorption of the fluids argon, carbon dioxide, hexafluoroethane, octafluoropropane, and decafluoropropane on a hydrophobic silicon wafer coated with octadecyltrichlorsilane by means of X-ray reflectivity (XRR), where we could access the supercritical regime for hexafluoroethane and argon. The XRR studies were carried out at PETRA III Beamline P08 (DESY, Hamburg) at a photon energy of 25 keV and Beamline BL9 (DELTA, Dortmund) at 27 keV, repsectively.

DS 4.12 Tue 10:00 P

Simulation Based Conductivity Tensor Determination of Sintered Nanosilver — •Lennart Schwan[1,2], Michael Feige[1], Andreas Hütten[2], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics, Interaktion 1, 33619 Bielefeld — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics, Universitätsstrasse 25, 33615 Bielefeld, Germany

3D-printing of conductive and dielectric materials in one process is an emerging technology. In addition to the printing of planar structures like circuit boards, the modern Multi Material Jetting process allows to realize three dimensional structures such as antennas, coils or cooling elements.

In the present case the conductive material consists of small silver particles which are sintered with infrared light. The conductivity reaches up to 70 % of the conductivity of copper but is highly anisotropic due to the print and sinter process.

In order to optimize the printed structures with regard to the anisotropic conductivity, it is necessary to determine reliable value of the conductivity tensor. Here we propose an approach based on a coupling of FEM simulation with mathematical optimization to determine the conductivity tensor. The simulation with the conductivity tensor as free parameter is fitted to experimental data of meander shaped test structures which are orientated in different directions to consider all components of the conductivity tensor.

DS 4.13 Tue 10:00 P

Molecular dynamics simulations of carbon nanomembranes (CNMs) — •Julian Ehrens, Levin Mihlan, 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 can not be adequately investigated by standard techniques, e.g. X-ray diffraction, which requires a characterization through physical quantities like solvent permeability and the Young's modulus. In order to propose possible internal molecular 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 use the experimental value of around 10 GPa for comparison. We present three distinct methods to calculate the Young's modulus: Global scaling of all coordinates (curvature of energy), stress-strain response from clamped straining and barostatted dynamics. Discrepancies among the methods with regard to vastly different outcomes of the Young's modulus will be discussed considering finite size effects and suitability of each method for this particular system.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" ChemPhysChem 21.10 (2020): 1006 [2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416

DS 4.14 Tue 10:00 P

Influence of processing parameters on the electrical conductivity of 3D printed silver structures — •Michael Feige, Lennart Schwan, and Sonja Schöning — Bielefeld Institute for Applied Materials Research (BIfAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics

3D-printing of conductive and dielectric materials in one process is an emerging technology. The Multi Material Jetting technique allows to realize three dimensional structures such as antennas, coils or cooling elements.

The deployed method is very similar to that used by a conventional inkjet printer. Small ink drops are deposited layer by layer through fine nozzles in the print heads. The stacking of those layers finally forms the 3D buildup. Multiple materials are introduced by two or more print heads.

In the considered case the dielectric material, a polymer, is cured with UV-light. The conductive material consists of small silver particles and is sintered with IR-light.

The electrical conductivity can reach up to 70 % of the conductivity of copper but it is anisotropic with regard to the print direction and it depends on several production parameters. We are identifying these contributing key factors, like layer thicknesses, drop placement patterns, environmental conditions during the print stage and temperature patterns used for heat treatment during postprocessing. In addition we investigate how the determined influence of the parameters can be used to optimize the conductivity.

DS 4.15 Tue 10:00 P

Selective Area Epitaxy of Bi-based 3D Topological Insulators on Sapphire — •Christoph Ringkamp, Michael Schleenvoigt, Peter Schüffelgen, Gregor Mussler, and Detlev Grützmacher — Peter-Grünberg-Institut 9, Forschungszentrum Jülich, 52428 Jülich, Germany

Topological insulators (TI) possess topologically protected, conducting surface states, which – in conjunction with superconductors (SC), are predicted to show Majorana signatures. A prerequisite for this is a high transparency between the TI and the SC, and that is why an in-situ fabrication of the TI/SC heterostructures is crucial. On Si(111) substrates, we have already established the selective area growth and a shadow mask technique to fabricate such heterostructures via molecular-beam epitaxy (MBE). However, one major problem in transport experiments still poses the impact of the Si substrate, as the Si/TI interface may serve as an additional conducting channel. Hence, we intend to grow the TI/SC heterostructures on sapphire, as it is a purely insulating substrate, which may allow to investigate the topological properties of the TI films in transport experiments in more detail.

We will report on the selective area epitaxy via MBE of Bi-based TI like Bi_2Te_3 and Bi_2Se_3 on sapphire substrates that are prepared with a combination of lithographically defined SiO_2 and Si_3N_4 structures as a growth mask and their application as a shadow mask for TI/SC heterostructures. Additionally, I will show a substantial improvement of the carrier mobility in the TI films on sapphire compared to Si(111).

DS 4.16 Tue 10:00 P

Area-selective deposition on 3D granular PtC scaffolds — •Fabrizio Porrati, Sven Barth, and Michael Huth — Goethe Uni Frankfurt

We present a novel fabrication method to prepare 3d metallic nanostructures by area-selective chemical vapor deposition (CVD). The

method is based on the fabrication of 3d PtC granular scaffolds by focused electron beam induced deposition (FEBID). These nanostructures are written between two electrods and biased by an electrical current in order to increase their temperature to several hundreds degrees. This is possible since the 3d PtC scaffolds are high ohmic resistors with low thermal coupling to the substrate. Here we show that CoFe and NbNC metallic layers form on the 3d biased scaffolds by decomposition of the HFeCo3(CO)12 and Nb(NMe2)3(N-t-Bu) precursor gas when injected in the SEM preparation chamber.

DS 4.17 Tue 10:00 P

Characterizing ALD printed structures by imaging ellipsometry — •Peter H. Thiesen[1], Ivan Kundrata[2,3], Maksym Plakhotnyuk[3], and Julien Bachmann[2,3] — [1]Accurion GmbH, Göttingen, Germany — [2]FAU, Erlangen, Germany — [3]ATLANT 3D, Lyngby, Dänemark

ATLANT 3D Nanosystems develops a disruptive 3D printing technology for micro and nano device rapid prototyping. The initial 3D printer prototype will be able to process oxides such as SiO2, TiO2, Al2O3, ZnO, and platinum with line width of 400 um. Later on, we will add processing of other materials, such as metals, sulfides, nitrides etc., also with a better selection of resolution down to 10 um. Thin film metrology of printed structures requires a fast measurement technique that is sensitive to thinnest films and offers a high lateral resolution also suited for the next development steps. Imaging Ellipsometry is an all-optical, non-contact metrology technique. It combines microscopic imaging with the measurement principles of spectroscopic ellipsometry and reaches a spatial resolution of about 1 micro meter. Ellipsometry is based on the samples interaction with polarized light and enables the characterization of ultra-thin films. The thickness of ALD-structures, printed at variable process parameters or with different materials was characterized by imaging ellipsometry. The standard characterization was done with a fixed angle of incidence system, equipped with a high power LED-HUB (SIMoN, EP4, Accurion GmbH) at an AOI of 60° and selected wavelength. Additionally, microscopic maps at different AOIs and wavelength of selected samples were recorded.

DS 4.18 Tue 10:00 P

Electrical transport properties of Vanadium-doped $Bi_2Te_{2.4}Se_{0.6}$ — Ch. Riha[1], B. Düzel[1], K. Graser[1], •O. Chiatti[1], E. Golias[2], J. Sánchez-Barriga[2], O. Rader[2], O. Tereshchenko[3], and S. F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Physics Department, Novosibirsk State University, 630090 Novosibirsk, Russia

Transport in the topological surface states (TSSs) of topological insulators, such as Bi_2Se_3, can be masked by unintentional bulk doping. The alloy $Bi_2Te_{2.4}Se_{0.6}$ is a promising candidate to investigate TSSs, because in $Bi_2Te_{3-y}Se_y$ materials bulk n-type doping tends to be suppressed. In this work [1], single crystals of $V_xBi_{2-x}Te_{2.4}Se_{0.6}$, with $x = 0.015$ and 0.03, are grown by the Bridgman method. Angle-resolved photoemission spectroscopy shows gapless TSSs for both Vanadium concentrations. The resistivity, the Hall charge carrier density, and the mobility for temperatures from 0.3 to 300 K are strongly dependent on the Vanadium concentration, with carrier densities as low as 1.5×10^{16} cm^{-3} and mobilities as high as 570 cm^2/Vs. Below 10 K, resistivity, carrier density, and mobility are constant, as expected for gapless TSSs. Also, the magnetoresistance shows for both Vanadium concentrations weak antilocalization, which is analyzed with the Hikami-Larkin-Nagaoka model and yields phase-coherence lengths of up to 250 nm for $x = 0.015$.

[1] C. Riha *et al.*, Phys. Status Solidi B, 2000088 (2020)

DS 4.19 Tue 10:00 P

Magnetotransport and thermoelectric properties of vanadium disulfide (VS_2) flakes — •Yejin Lee[1,2], Gyu-Hyeon Park[1,2], Grigory Shipunov[1], Geishendorf Kevin[1], Bernd Buechner[1], Kornelius Nielsch[1,2], Saicharan Aswatham[1], and Andy Thomas[1,2] — [1]IFW Dresden — [2]Technische Universität Dresden

Two-dimensional transition metal dichalcogenides (TMDCs) have drawn extensive interest due to their intriguing electrical transport properties. Vanadium disulfide (VS_2) is a member of metallic TMDCs and interestingly, theoretical calculations have predicted magnetic characteristics. Here, we investigate magnetotransport and thermoelectric properties of exfoliated VS_2 flakes from a single crystal grown by chemical vapor transport technique. The magnetotransport characterizations were performed in an external magnetic field of up to 9 T. We found that the VS_2 flake exhibits a specific temperature dependence at around 21 K, which is consistent with the presence of a weak magnetic anomaly seen in the single crystal. In addition, a negative magnetoresistance is observed with a steep decrease at 2.5 T and below 20 K, where the slope of the magnetic field dependent Hall resistance changes. Furthermore, Seebeck coefficients are evaluated and it indicates a p-n type transition in the low temperature regime if a single band model is assumed. This findings provide further insight into the magnetotransport and thermoelectric properties of van Der Waals TMDCs.

DS 4.20 Tue 10:00 P

Influence of the module number on the folding process in thin spider silk films — •Mirjam Hofmaier[1,3], Birgit Urban[1], Sarah Lentz[4], Thomas Scheibel[4], Andreas Fery[1,3], and Martin Müller[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden — [2]Technical University Dresden, Chair of Macromolecular Chemistry, 01062 Dresden — [3]Technical University Dresden, Chair of Physical Chemistry of Polymeric Materials, 01062 Dresden — [4]University of Bayreuth, Chair of Biomaterials, Prof.-Rüdiger-Bormann Str. 1, 95447 Bayreuth

Aiming at a better understanding of the folding process in recombinantly produced[1], multiblockcopolymer-like spider silks, herein we report experimental work on thin films of eADF4(Cx) proteins with x = 1-16 modules. Thin eADF4(Cx) films were characterized as-cast and during methanol post-treatment (pt) using dichroic attenuated total reflection (ATR-) FTIR spectroscopy, circular dichroism (CD), and scanning force microscopy (SFM).[2]

During post-treatment, FTIR reveals an increasing β-sheet content from $< 10\%$ to > 28 % and a decreasing random coil content from $> 65\%$ to $< 50\%$, which could be confirmed by CD analysis.[2-3] An out-of-plane orientation of the antiparallel β-sheets of the crystalline blocks could be suggested by dichroic ATR-FTIR spectroscopy.[2]

[1] D. Huemmerich et al., Biochem., 2004, 43, 13604-13612. [2] M. Hofmaier et al., JPC B, 2021, 125, 1061-1071. [3] C. Borkner et al., ACS Appl. Polym. Mater., 2019, 1, 3366-3374.

DS 4.21 Tue 10:00 P

Enhancement of the Raman Emission in Hexagonal Boron Nitride — •Felix Schaumburg, Marcel Ney, Vasilis Dergianlis, Günther Prinz, Martin Paul Geller, and Axel Lorke — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Optical spectroscopy, especially Raman- and photoluminescence (PL)-spectroscopy, is commonly used to study the optical properties of two-dimensional materials. In order to obtain the highest signal, it is important to reduce spurious effects, such as backscattered laser light.

We studied a number of exfoliated h-BN flakes with different thicknesses on a silicon (Si) substrate with a 300 nm silicon dioxide (SiO_2) top-layer. With changing the h-BN layer-thickness, we found a specific thickness, where all Raman signals showed maximum intensity, whereas the backscattered laser light was almost completely suppressed. To explain the increased signal, we calculated the reflectivity of the layer system (air, h-BN, SiO_2, Si) for different h-BN layer thickness, by using the transfer-matrix-algorithm. For our 532 nm excitation laser, the minimum surface reflectivity was found for a layer thickness of around 160 nm. With AFM measurements, we were able to confirm that the thickness of the samples, with the strongest Raman signal, corresponds almost exactly to the calculated thickness.

Our results suggest that the PL from defects will also be strongly enhanced for an h-BN thickness of 160 nm and an excitation laser wavelength of 532 nm. This optimal thickness for the defect state PL emission can easily be calculated for other excitation laser wavelengths, as well as for other materials.

DS 4.22 Tue 10:00 P

Vibrational spectroscopic characterization of local electrochemical modification of graphene — Tilmann Neubert[1,2,3,4], Jörg Rappich[1], Kannan Balasubramanian[3,4], and •Karsten Hinrichs[2,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489, Berlin — [2]ISAS - e.V., In Situ Spectroscopy Group, Schwarzschildstr. 8, 12489 Berlin — [3]HU Berlin, School of Analytical Sciences Adlershof (SALSA), Unter den Linden 6, 10117 Berlin — [4]Department of Chemistry, HU Berlin, Unter den Linden 6, 10117 Berlin

Local properties of an electrochemical modification and the underlying graphene between the contacts of a field effect transistor (FET) were analyzed by Raman and infrared (IR) spectroscopies. IR spectroscopic ellipsometry (IRSE) enabled us to probe spots from about 0.1 to a few mm, IR microscopy of a few 10 μm, Raman of about 1 μm, photothermal AFM-IR at the nm-scale. For graphene surfaces modified electrochemically with maleimidophenyl (MP) or 4-Aminophenyl acetic acid (4-APhAA) the interpretation of Raman spectra allowed a detailed characterization of the graphene properties whereas IR is used for identification of characteristic molecular vibrations of the functional layers. The Raman spectra reveal if the electrochemically formed oligomers are covalently bound or physically adsorbed. AFM-profiles and IRSE interpretation reveal similar thicknesses of the deposited (a few nm thick) layers. Funding: EFRE 1.8/13 and SALSA.

DS 4.23 Tue 10:00 P

The Dielectric Tensor of Microtextured Squaraine Thin Films obtained by Imaging Mueller Matrix Ellipsometry — •Manuela Schiek[1], Sebastian Funke[2], Matthias Duwe[2], Peter H. Thiesen[2], Kurt Hingerl[1], and Frank Balzer[3] — [1]Johannes Kepler University of Linz, Austria. — [2]Accurion GmbH Göttingen, Germany. — [3]University of Southern Denmark, DK.

Imaging Mueller matrix ellipsometry combines the power of variable angle spectroscopic ellipsometry and optical microscopy mapping. Here we illustrate the determination of the full biaxial dielectric tensor of an organic material crystallizing in an orthorhombic phase. This is achieved by analyzing thin film samples with a single crystallographic orientation parallel to the substrate subdivided in micro-sized rotational domains. Oscillator dispersion relations reasonably model the diagonal tensor components and reproduce well the Davydov splitting of the material.

[1] Funke, Duwe, Balzer, Thiesen, Hingerl, Schiek. J. Phys. Chem. Lett. 19 (2021) 3053.

DS 4.24 Tue 10:00 P

Modelling of Two-Dimensional Electronic Spectroscopy Response of a Plasmon-Exciton System — •Marti Bosch[1], Antonietta De Sio[2], Christoph Lienau[2], and Erich Runge[1] — [1]TU Ilmenau — [2]Universität Oldenburg

Two-dimensional electronic spectroscopy (2DES) records the optical response of a system after the interaction with three timely delayed laser pulses. The dynamics and electronic couplings in complex optical systems can be analyzed with a high temporal resolution by correlating the excitation and emission intensities as a function of the time delay as well as the used frequencies. The interpretation of 2DES experimental results is challenging and it is often useful to support them with numerical calculations. In this work, we present the semiclassical calculations of the third order non-linear response signal of a plasmon-exciton system. We model the response signal of coupled two-level systems based on a perturbative density matrix approach [1] and implement the non-unitary time evolution of the system using the Lindblad formalism. We discuss the differences appearing for fermionic and bosonic systems and compare the results to preliminary experimental results. [1] Mukamel, S. (1995) Principles of nonlinear optical spectroscopy. O.U.P, New York

DS 4.25 Tue 10:00 P

Surface-localized phonon modes on the Si(553)-Au surface — •Julian Plaickner[1,2], Eugen Speiser[1], Sandhya Chandola[1,2], Christian Braun[3], Wolf Gero Schmidt[3], Norbert Esser[2,4], and Simone Sanna[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn Meitner Platz 1, 14109 Berlin — [2]Leibniz-Institut für Analytische Wissenschaften, ISAS e.V., Schwarzschildstraße 8, 12489 Berlin — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn — [4]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin — [5]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus Liebig Universität Gießen, Heinrich Buff Ring 16, 35392 Gießen

The Si(553)-Au surface is investigated with Raman spectroscopy and ab-initio calculations. A characterization of the phonon modes is provided below and above the phase transition temperature (Phys. Rev. B 103, 115441 (2021)). Some phonon modes shows a significant temperature dependence. The analysis of the calculated displacement patterns indicates that these modes are localized at the Si step edge or involve a change of the Au-Au bond length. The large temperature-induced frequency shift observed for transversal Au-related modes demonstrates that the dimerization is significantly affected by the phase transition due to charge transfer between Au- and Si-related states. The charge transfer leads to Raman scattering by charge density fluctuations, which is responsible for the detected Raman activity even for such modes that should be silent due to symmetry.

DS 4.26 Tue 10:00 P

Femtosecond Spectrostroscopic Ellipsometry — •Shirly Espinoza — ELI Beamlines, Institute of Physics, Czech Academy of Science, Prague, Czech Republic

The current status of a versatile experimental platform dedicated to ultrafast pump-probe ellipsometry with time resolution about 100 fs will be presented. The setup measures the ellipsometric spectra in the range 350-750 nm. The monochromatic pump beam can be chosen from 350 nm to 2 um. This setup give information of ultrafast changes on the optical properties of the materials forming a thin film. Recent results and ideas for expansion of the capabilities of the setup will be presented for discussion.

DS 4.27 Tue 10:00 P

Metal-insulator transition via ion irradiation in epitaxial La0.7Sr0.3MnO3-δ thin films — Lei Cao[1], Andreas Herklotz[2], Diana Rata[2], Chenyang Yin[3], Oleg Petracic[3], Ulrich Kentsch[1], Manfred Helm[1], and •Shengqiang Zhou[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, 01328, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, 06120, Germany — [3]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH Jülich, 52425, Germany

Complex oxides provide rich physics related to ionic defects. For the proper tuning of functionalities in oxide heterostructures, it is highly desired to develop fast, effective and low temperature routes for the dynamic modification of defect concentration and distribution. In this work, we report on the use of helium-irradiation to efficiently control the vacancy profiles in epitaxial La0.7Sr0.3MnO3-δ thin films. The viability of this approach is supported by the lattice expansion in the out-of-plane lattice direction and dramatic change in physical properties, i.e., a transition from ferromagnetic metallic to antiferromagnetic insulating. In particular, a significant increase of resistivity up to four orders of magnitude is evidenced at room temperature, upon irradiation by highly energetic He-ions. Our result offers an attractive means for tuning the emergent physical properties of oxide thin films, via strong coupling between strain, defects and valence.

The work at HZDR is supported by DFG (ZH 225/10-1).

DS 5: Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Tuesday 13:30–16:15 Location: H3

Topical Talk DS 5.1 Tue 13:30 H3

Single crystal diamond grown by CVD: state of the art, current challenges and applications — •Jean-Charles Arnault[1], Samuel Saada[2], and Victor Ralchenko[3,4] — [1]NIMBE, UMR CEA-CNRS 3685, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CEA, LIST, DM2I, F-91191 Gif-sur-Yvette, France — [3]Prokhorov General Physics Institute of Russian Academy of Sciences, Vavilov str. 38, Moscow 119991, Russia — [4]Harbin Institute of Technology, Harbin 150080, P.R. China

Single crystal diamond is the material of choice for future power electronics. Its electrical and thermal properties outperform those of other wide band gap semiconductors like 4H-SiC, GaN or Ga2O3. In addition, diamond can host a wide range of color centers (NV, SiV, GeV,...) that bring optical and spin properties suitable for quantum applications. This explains the ultrafast development of quantum applications based on diamond materials within the last years. For both application fields, diamond films of excellent crystalline quality are required and an accurate tuning of dopants is needed. This talk will draw the state of art of single crystal diamond grown by CVD either starting with diamond substrate (homoepitaxy) or controlling diamond epitaxial nucleation on a foreign substrate (heteroepitaxy). Progresses on substrates, growth mechanisms and reduction of structural defects, doping, upscaling and applications will be reviewed. In light of last progresses, future challenges and the respective roles of homoepitaxial and heteroepitaxial materials in the applications roadmap will be discussed.

Topical Talk DS 5.2 Tue 14:00 H3

Tuning Semiconductor Mode-Locked Laser Frequency Combs by Gain and Cavity Design — Stefan Meinecke and •Kathy Lüdge — Institute of Theoretical Physics, Technische Univ. Berlin

Passively mode-locked semiconductor lasers produce sequences of short optical pulses at high repetition rates without the need for an external driving frequency. They find applications in optical data communication and metrology and are promising candidates for comb generation in all-optical integration schemes [1].

The gain material as well as the cavity design play a crucial role for their performance and can be designed easily via epitaxial growth. We explore the pulse performance optimization of a three-section tapered quantum-dot laser by means of a numerical model that assumes both the microscopic charge-carrier scattering processes as well as the light-propagation along the device. Motivated by an experimentally characterized device [2], we utilize pulse peak power, pulse width and long-term timing jitter to characterize the performance. The results predict optimal configurations for both the angle of the tapered gain section and the position of the saturable absorber section. These findings can be interpreted and understood in terms of the gain and absorption recovery processes within the active regions of the laser and thus explain why the nano-structured quantum-dot gain medium is especially suited for optimizing the pulse performance.

[1] R. Guzmán et al., Opt. Lett. 42, 2318 (2017).
[2] S. Meinecke et al., Sci. Rep. 9, 1783 (2019).

Topical Talk DS 5.3 Tue 14:30 H3

Monolayer-thick GaN/AlN heterostructures for UVB & UVC ranges: technology, design and properties — Valentin Jmerik, Alexey Toropov, Valery Davydov, and •Sergey Ivanov — Ioffe Institute, Polytekhnicheskaya 26, Saint Petersburg, 194921, Russia

The development of monolayer (ML)-thick GaN/AlN multilayer heterostructures for deep ultraviolet (UV) optoelectronics is discussed. Analysis of plasma-assisted molecular beam epitaxy and metal-organic vapor phase epitaxy show that extreme interface sharpness and sub-ML accuracy in controlling the layer thickness are the main advantages of the former, while the lowest density of threading dislocations and wide possibilities for the implementation of various two-dimensional growth mechanisms are the attractive features of the latter. The structural properties of ML GaN/AlN heterostructures are evaluated comparatively by X-ray diffraction, scanning transmission electron microscopy and Raman spectroscopy. Studies of the optical properties of ML-thick GaN/AlN quantum wells (QWs) reveal that quenching of the Stark effect, suppression of polarization switching, as well as a true excitonic nature of the UV-emission in ultra-thin (1-2ML) QWs ensure a high internal quantum yield of 75% in such structures emitting at 235 nm. High optical quality of 100-nm-thick layers of ML-GaN/AlN digital alloys is confirmed by the optically pumped stimulated emissions in the range 262-290 nm with a minimum threshold of 700kW/cm2. The possibilities of using ML-GaN/AlN MQWs to fabricate powerful (Watt-range) electron-beam pumped UVC-emitters in the spectral range 240-260 nm are demonstrated.

15 minutes break

Topical Talk DS 5.4 Tue 15:15 H3

Optical and vibrational properties of layered 2D materials — •Janina Maultzsch — Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Atomically thin layered crystals have received great attention due to their fascinating physical properties. By deterministic stacking and twisting of these two-dimensional (2D) materials, an almost unlimited variety of material's combinations and resulting physical properties can be achieved. The properties can be further modified by chemical functionalization of the surface. In this talk I will present theoretical predictions on novel 2D antimony oxide structures which show tunable electronic properties depending on the oxygen content. Second, based on recent experiments on chemically functionalized MoS_2 layers,

we present transitions from the 2H to the 1T' phase along with the characteristic phonon modes of the 1T' phase of MoS_2.

Topical Talk DS 5.5 Tue 15:45 H3
Organic/inorganic low dimensional material systems: Fundamental aspects and device applications — •Emil List-Kratochvil — Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany — Helmholtz-Zentrum für Materialien und Energie GmbH, HySPRINT Helmholtz Innovation Lab, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The ability to form heterostructures from different materials, yet from the same material class, has revolutionized electronic and optical technologies during the past decades. To explore novel electronic and optoelectronic functionalities based on heterostructures in a natural next step we have turned to systematically explore hybrid inorganic/organic materials systems (HIOS) in heterostructures combining materials from dissimilar material classes. Among different aspects in this HIOS research endeavour, it was found that an in-depth understanding and control over the energy level alignment in HIOS is the key to attain novel electronic and optoelectronic functionalities. In this contribution, we report on fundamental aspects of the self-assembled monolayer formation on different metal oxide and 2D semiconductors such as transition metal dichalcogenides, observations of switching processes and successful implementations in diode, light emitting diode, electrolyte gated field effect transistor and neuromorphic plasmonic device structures.

DS 6: Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)

Topological insulators are a striking example of materials in which topological invariants are manifested in robustness against perturbations. Topology has emerged as an abstract, yet surprisingly powerful, new paradigm for controlling the flow of an excitation, e.g. the flow of electrons or light. This interdisciplinary Focus Session aims at discussing the latest experimental and theoretical results in the fast developing field of topological phenomena in synthetic matter. The recent merging of topology and cold atoms, photonics, mechanics and many more fields promises a considerable impact on these disciplines. We bring together leading theoretical and experimental experts from the fields of topological phenomena in synthetic matter to discuss recent progress and interdisciplinary synergy emerging at the interface of these fields. Furthermore, we give an overview to young scientists of exciting possibilities of interdisciplinary research in these fields with the special focus on the practical applications of fundamental science.

Organizer: Sebastian Klembt (Julius-Maximilians-Universität Würzburg)

Time: Thursday 13:30–16:15 Location: H1

Topical Talk DS 6.1 Thu 13:30 H1
Exceptional Topology of Non-Hermitian Systems: from Theoretical Foundations to Novel Quantum Sensors — •Jan Carl Budich — Institute of Theoretical Physics, TU Dresden, Dresden, Germany

In a broad variety of physical settings ranging from classical metamaterials to open quantum systems, non-Hermitian (NH) Hamiltonians have proven to be a powerful and conceptually simple tool for effectively describing dissipation. Motivated by recent experimental discoveries, investigating the topological properties of such NH systems has become a major focus of current research. In this talk, I give a brief introduction to this rapidly growing field, and present our latest results. Specifically, we discuss the occurrence of novel topological phases unique to NH systems. There, the role of spectral degeneracies familiar from Hermitian systems such as Weyl semimetals is played by exceptional points at which the effective NH Hamiltonian becomes non-diagonalizable. Furthermore, we show how guiding principles of topological matter such as the bulk boundary correspondence are qualitatively changed in the NH realm. Finally, we demonstrate that the sensitivity of NH systems to small changes in the boundary conditions may be harnessed to devise novel high-precision sensors.

Topical Talk DS 6.2 Thu 14:00 H1
In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices — •Peter Schüffelgen — Forschungszentrum Jülich

With their experimental verification in 2007, topological insulators render a new and fascinating material class. A band inversion in the bulk of a 3D topological insulator creates a 2D metallic Dirac system at the physical surface of those 3D crystals. The surface Dirac states are topologically protected and have their spin locked to their momentum. This intrinsic quantum spin texture promises to enable fundamentally new, yet elusive quantum technologies, such as Majorana quantum bits. In this talk, I will introduce the material class of (Bi,Sb)-based topological insulators and discuss experimental challenges. I will present an in situ process that makes it possible to construct hybrid devices comprised of topological and superconductive nanostructures fully under ultra-high vacuum conditions via molecular beam epitaxy. A combination of stencil lithography and selective area growth allows for the realization of a variety of superconductor-topological insulator hybrid devices and solves the associated fabrication challenges.

Topical Talk DS 6.3 Thu 14:30 H1
Atomic monolayers as two-dimensional topological insulators — •Ralph Claessen — Physikalisches Institut und Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Two-dimensional topological insulators (2D-TIs) are characterized by hosting spin-polarized conducting band states at their one-dimensional (1D) edges, giving rise to the quantum spin Hall (QSH) effect. As pointed out in the seminal work of Kane and Mele, graphene would constitute the most simple realization of a QSH insulator if it were not for its almost negligible spin-orbit interaction. It has been suggested that going to heavier group IV monolayers (such as the Sn-derived "stanene") could remedy this problem, but a convincing demonstration of such 2D TIs is still lacking. Recently we discovered that the neighboring groups III and V in the Periodic Table provide a promising alternative. Here I will discuss rational design, epitaxial synthesis, as well as ARPES and STM studies of two such synthetic QSH insulators, namely Bi (bismuthene) and In (indenene) monolayers grown on SiC(0001) substrates.

15 minutes break

Topical Talk DS 6.4 Thu 15:15 H1
Topological Insulator Lasers — •Mordechai Segev — Technion - Israel Institute of Technology

Topological Insulator Lasers are semiconductor emitters fabricated on a potential landscape designed to harness the features of topological insulators to force injection-locking of the emitters, making them act as a single coherent laser. The concepts underlying topological insulator lasers will be reviewed along with the recent progress.

Topical Talk DS 6.5 Thu 15:45 H1
TBA — •Morais Smith — TBA

TBA

DS 7: Thin Oxides and Organic Thin Films (joint session DS/CPP)

Time: Thursday 15:15–16:15 Location: H5

DS 7.1 Thu 15:15 H5

Hybrid electronic states in epitaxially layered perovskite oxide electrocatalysts for water electrolysis — •Lisa Heymann[1], Moritz Weber[1], Marcus Wohlgemuth[1], Felix Gunkel[1], and Christoph Baeumer[1,2] — [1]Peter Gruenberg Institute and JARA-FIT, Forschungszentrum Juelich GmbH, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

In electrochemical water splitting catalyzed by perovskite oxides (ABO_3), the B-O hybridization degree has a major impact on the electrocatalytic activity. Additionally, space charge layers at the interface to the electrolyte may hamper the electron transfer into the electrode, complicating the analysis of hybridization phenomena. The goal in this work was to explore whether A site doping in cobaltites ($ACoO_3$) has a major impact on the oxygen evolution reaction (OER) through a different degree of hybridization or the extend of a surface space charge layer. We investigated $La_{0.6}Sr_{0.4}CoO_3$ and $LaCoO_3$ bilayer structures in epitaxial thin films that enabled us to create a near surface depth profile of both, the hybridization degree and the doping concentration confirmed by x-ray photoelectron spectroscopy (XPS). In a Mott Schottky (MS) analysis, we showed that in the OER potential regime the catalytic activity is not limited by a space charge layer. Therefore, we can correlate the observed OER activity trend to the degree of hybridization in cobaltites. The combined XPS and MS analysis enables to differentiate between the influence of the hybridization degree and intrinsic space charge layers, which are indistinguishable in a sole physical or electrochemical characterization.

DS 7.2 Thu 15:30 H5

tailored electrical characteristics in TiOx/HfOx-based memristive device for targeting neuromorphic computing — •Seongae Park[1,2], Stefan Klett[1], Tzvetan Ivanov[1,2], Andrea Knauer[2], Joachim Doell[2], and Martin Ziegler[1,2] — [1]Department of Electrical Engineering and Information Technology, TU Ilmenau, Ilmenau, Germany — [2]Institute of Micro and Nanotechnologies MacroNano, TU Ilmenau, Ilmenau, Germany

Over the last few years, memristive devices have shown their high potential for neuromorphic computing. In particular, redox-based memristive devices have become the focus of research interest, since they enable precise emulation of synaptic functionality through local ionic processes. However, for targeted device functionality, a detailed understanding of ionic processes at the atomic level is required, which is often severely hampered by coupled electronic and ionic processes. In this talk, the bi-layer oxide system TiOx/HfOx is presented. In a combined approach using a 4-inch wafer process technology and a physical device model, we show the contribution of physical device parameters such as device area size, the thickness of HfOx, interface modification, as well as the stoichiometry of HfOx to the electrical characteristics. Furthermore, we present how those parameters can be tuned for customized device functionalities. In that respect, memristive devices with tailored I-V characteristics and analog resistive switching are obtained that own an intrinsic self-compliance and do not need electroforming-free cycles.

DS 7.3 Thu 15:45 H5

Arrangement and electronic properties of cobalt phthalocyanine molecules on Si(111) ($\sqrt{3}\times\sqrt{3}$) R30°-B — •Milan Kubicki, Martin Franz, Susi Lindner, Holger Eisele, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject because of their possible application in advanced optical and electronic devices. Here, the molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated Si(111) ($\sqrt{3}\times\sqrt{3}$) R30°-B surface are studied by scanning tunneling microscopy and spectroscopy [1,2]. It is found that for submonolayer coverages the CoPc molecules lie flat on the Si surface with the Co d_{z^2} orbital of the molecule forming a hybrid state with the p_z orbital of the Si adatom at the surface. For multilayer coverages in contrast, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films, and the electronic properties resemble those of pure CoPc.

[1] S. Lindner, M. Franz, M. Kubicki, S. Appelfeller, M. Dähne, and H. Eisele, Phys. Rev. B **100**, 245301 (2019).

[2] M. Kubicki, S. Lindner, M. Franz, H. Eisele, and M.Dähne, J. Vac. Sci. Technol. B **38**, 042803 (2020).

DS 7.4 Thu 16:00 H5

Experimental Quantification of Interaction Energies in Organic Monolayers — •Pierre-Martin Dombrowski, Stefan Renato Kachel, Leonard Neuhaus, Tobias Breuer, J. Michael Gottfried, and Gregor Witte — Philipps-Universität Marburg, Germany

The formation of molecular nanostructures is determined by the interplay of intermolecular and molecule-substrate interactions. However, these interactions are experimentally hardly accessible. Temperature-programmed desorption (TPD) is a fairly well-established experimental technique capable of quantifying both types of interaction, but its quantitative analysis is by no means trivial. In the present study, we analyse the desorption kinetics of the two organic semiconductors pentacene (PEN) and perfluoropentacene (PFP) from Au(111) and MoS_2 surfaces to show the potential of TPD, but also highlight challenges for large adsorbates. Combining TPD with scanning tunnelling microscopy, work function measurements and theoretical modelling, we show that intermolecular interactions are dominated by the intramolecular charge distribution, resulting in net intermolecular repulsion in unitary and attractive interactions in mixed PEN:PFP monolayers. We determine the coverage-dependent prefactor of desorption with unprecedented precision and correlate its evolution with the activation of specific degrees of freedom of motion of adsorbed molecules. Lastly, we compare differences in molecule-substrate interactions on Au(111) and MoS_2, revealing that (sub-)monolayers on MoS_2 are stabilized only by entropy.

DS 8: Annual General Meeting of the Thin Films Division

Time: Thursday 18:00–19:00 Location: MVDS

Annual General Meeting

DS 9: Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Friday 10:00–11:00 Location: H1

DS 9.1 Fri 10:00 H1

Additive manufacturing of permanent magnets based on $(CoCuFeZr)_{17}Sm_2$ — •Dagmar Goll, Felix Trauter, Philipp Braun, Judith Laukart, Ralf Löffler, Ute Golla-Schindler, and Gerhard Schneider — Aalen University, Materials Research Institute, Beethovenstr. 1, 73430 Aalen, Germany

Lab-scale additive manufacturing of $(CoCuFeZr)_{17}Sm_2$-based powder was performed to realize CoSm printed parts with hard magnetic properties. For manufacturing a special inert gas process chamber for laser powder bed fusion was used. A three-step annealing procedure analogous to sintered magnets was applied. This led to a coercivity of 2.77 T, remanence of 0.78 T and maximum energy density of 109.4 kJ/m^3 for the printed parts. Compared to an isotropic sintered magnet of comparable composition and annealing procedure, the coercivity is of the same order. Due to the texture of the printed parts the remanence is 24 % larger.

DS 9.2 Fri 10:15 H1

Structure solution of a large unit cell approximant derived from $SrTiO_3$ on Pt(111) — •Stefan Förster[1], Sebastian Schenk[1], Oliver Krahn[1], Holger L. Meyerheim[2], Marc DeBoissieu[3], and Wolf Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Universite Grenoble Alps, CNRS, SIMaP, Saint-Martin d'Hères, France

The discovery of two-dimensional oxide quasicrystals (OQC) has caused a great amount of interest in aperiodic structure formation from perovskite materials on metal surfaces [1]. In recent years, a plethora of surface science techniques has been applied to OQCs to get an understanding of this peculiar materials system on the fundamental level [2]. In this contribution, we present low-temperature scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) investigation of the largest unit cell approximant known so far in 2D systems. Its unit cell covers an area of approximately 44 Å × 44 Å and has p2gg symmetry. STM measurements show 48 atoms in the unit cell forming the vertices of 48 triangles, 18 squares and 6 rhombuses. The structure has been solved utilizing over 300 independent reflections measured by SXRD with an R-factor better than 0.20. From this analysis a profound understanding of the decoration of all tiles with Sr, Ti, and O ions is derived, which solves the structure of the parent OQC.
[1] S. Förster et. al., Nature 502, 215 (2013).
[2] S. Förster et al., Phys. Status Solidi B 257, 1900624 (2020).

DS 9.3 Fri 10:30 H1

Surface reconstructions: challenges and opportunities for the growth of perovskite oxides — Giada Franceschi, Michael Schmid, Ulrike Diebold, and •Michele Riva — Institute of Applied Physics, TU Wien, Austria

Achieving atomically flat and stoichiometric films of complex multicomponent oxides is crucial for integrating these materials in emerging technologies. While pulsed laser deposition (PLD) can in principle produce these high-quality films, experiments often show rough surfaces and nonstoichiometric compositions.

To understand the cause, we follow the growth at the atomic scale from its early stages, using STM. We focus on $SrTiO_3$(110) and $La_{0.8}Sr_{0.2}MnO_3$(110) films. For both, the non-stoichiometries introduced during growth accumulate at the surface. As a result, their surface structure evolves along phase diagrams of surface structure vs. composition [1,2,3]. This can drastically degrade the surface morphology: pits develop on reconstructed areas with different sticking [4]; ill-defined oxide clusters nucleate when the non-stoichiometry introduced is too large to be accommodated in the surface by changing its structure. On the flip side, one can take advantage of the high sensitivity of surface structures to composition deviations to grow films with thickness of several tens of nanometers retaining atomically flat surfaces, and with stoichiometry control better than 0.1% [1].
[1] Phys. Rev. Mater. **3**, 043802 (2019). [2] J. Mater. Chem. A **8**, 22947 (2020). [3] arXiv:2010.05205 (2020). [4] Phys. Rev. Res. **1**, 033059 (2019).

DS 9.4 Fri 10:45 H1

Investigation of Spin Pumping through α-Sn Interlayer — •Leszek Gladczuk[1], Lukasz Gladczuik[2], Piotr Dluzewski[1], Gerrit van der Laan[3], and Thorsten Hesjedal[2] — [1]Institute of Physics, Polish Academy of Science — [2]Department of Physics, Clarendon Laboratory, University of Oxford — [3]Diamond Light Source, Harwell Science and Innovation Campus

Elemental tin in the α-phase is an intriguing member of the family of topological quantum materials. In thin films, with decreasing thickness, α-Sn transforms from a 3D topological Dirac semimetal (TDS) to a 2D topological insulator (TI). Getting access to and making use of its topological surface states is challenging and requires interfacing to a magnetically ordered material. Recently we have successfully performed an epitaxial growth of α-Sn thin films on Co, forming the core of a spin-valve structure, is reported. Time- and element-selective ferromagnetic resonance experiments were conducted to investigate the presence of spin pumping through the spin-valve structure. A rigorous statistical analysis of the experimental data using a model based on the Landau-Lifshitz-Gilbert-Slonczewski equation was applied. A strong exchange coupling contribution was found, however no unambiguous proof for spin pumping. Nevertheless, the incorporation of α-Sn into a spin valve remains a promising approach given its simplicity as an elemental TI and its room-temperature application potential.

DS 10: Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)

Time: Friday 11:15–13:00 Location: H1

DS 10.1 Fri 11:15 H1

Free-Standing ZnSe-Based Microdisk Resonators - Influence of Edge Roughness on the Optical Quality and Degradation Reduction with Supported Geometry — •Wilken Seemann[1], Alexander Kothe[1], Christian Tessarek[1], Gesa Schmidt[2], Siqi Qiao[2], Nils von den Driesch[2], Jan Wiersig[3], Alexander Pawlis[2], Gordon Callsen[1], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Institut für Physik, Universität Magdeburg, Germany

Free-standing microdisks with ZnCdSe quantum wells in ZnMgSe barriers are analyzed using micro-photoluminescence (μPL). Stimulated emission into whispering gallery modes (WGMs) is demonstrated. Deformation functions of the resonators are determined via scanning electron microscopy (SEM). A correlation between edge roughness and optical quality is found. These results are confirmed by calculations based on the boundary element method using the measured deformation functions.

To reduce degradation in the ZnSe structures a fabrication technique new to this material system is introduced. It yields "supported" disks with no underetching which enhances the mechanical stability of the resonator and its thermal contact to the substrate. SEM measurements reveal an excellent structural quality of these resonators. The formation of WGMs in supported ZnSe:Cl resonators is demonstrated in μPL and confirmed by theoretical calculations.

DS 10.2 Fri 11:30 H1

Pyramid formation by etching of InGaN/GaN quantum well structures grown on N-face GaN for nano optical light emitters — •Uwe Rossow, Savutjan Sidikejiang, Samar Hagag, Philipp Henning, Rodrigo de Vasconcellos Lourenco, Heiko Bremers, and Andreas Hangleiter — TU Braunschweig, Inst. f. Angewandte Physik

While growth processes of $In_xGa_{1-x}N$/GaN quantum well structures on the Ga-face of GaN buffer layers are already optimized to obtain high quantum efficiency, the growth on N-face has gained momentum only in the last years. Compared to Ga-face $In_xGa_{1-x}N$ layers are more stable on N-face and the surface can easily be structured by wet chemical etching, which usually leads to the formation of pyramids on the surface. This allows a new way to realize nano optical light emitters which offers the possibility to produce structures with similar emission properties. First we grow $In_xGa_{1-x}N$/GaN (single or multi) quantum well structures on N-face GaN. In a second step pyramids are formed by KOH etching. We demonstrate that pyramids with smooth side facets of the type $(1\bar{1}0\bar{1})$ and sharp tips in the nanometer range can be achieved without any sign of damage. TEM reveals that InGaN quantum dot-like structures are present in the pyramids and in photoluminescence narrow emission lines are observed. The etching process depends on electrolyte composition and temperature, defects at the surface and surface morphology. A better control of this process is required to achieve reproducible nano structures.

DS 10.3 Fri 11:45 H1

Bulk and interfacial effects in the Co/Ni_xMn_{100-x} exchange-bias system due to creation of defects by Ar^+ sputtering — •Tauqir Shinwari[1], Ismet Gelen[1], Yasser A. Shokr[1,2], Ivar Kumberg[1], Ikram Ullah[3], Muhammad Sajjad[3], M. Yaqoob Khan[3], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Arnimallee 14, Berlin 14195, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt — [3]Department of Physics, Kohat University of Science and Technology, Kohat, Khyber Pakhtunkhwa 26000, Pakistan

A series of experiments is carried out to identify the contribution of interface and bulk antiferromagnetic (AFM) spins to exchange bias (EB) in ultrathin epitaxial ferromagnetic (FM)/AFM bilayer samples. These are single-crystalline AFM Ni_xMn_{100-x} and FM Co layers on $Cu_3Au(001)$, in which structural or chemical defects are introduced by controlled Ar^+ sputtering at the surface of the AFM layer or at a certain depth inside the AFM layer. Comparison of the magnetic properties measured by magneto-optical Kerr effect for sputtered and non-sputtered parts of the same sample then allows a precise determination of the influence of sputtering on the AFM layer during the sample preparation. The results show that the creation of defects in the bulk of the AFM layer enhances the magnitude of EB and its blocking temperature, but not the ones at the interface. We also observed that the deeper the insertion of defects in the AFM layer, the higher the EB field and the larger the coercivity. These findings are discussed as the effect of additional pinning centers in the bulk of the AFM layer.

DS 10.4 Fri 12:00 H1

Study of annealing effect on RF-sputtered Bi2Te3 thin films with full figure of merit characterization. — •Gyuhyeon Park, Maksim Naumochkin, Kornelius Nielsch, and Heiko Reith — Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

Thermoelectric (TE) devices enable the direct conversion of heat into electricity and vice versa. The demand of micro TE harvesting or Peltier cooling devices for application in autonomous sensor systems required for the internet of things (IoT) will prospectively drastically increase in the coming years. Such microdevices are typically fabricated using electrodeposition or physical vapor deposition, where the successful optimization of the thermoelectric figure of merit, zT, which is the key enabler for the introduction of these devices to application. Accordingly, thin film fabrication methods and material investigation are of high interest. In this study, we report on the thermoelectric characterization of RF sputtered n-Bi2Te3 thin films with various thicknesses. For the in-plane Seebeck coefficient, Hall coefficient, electrical, and thermal conductivity measurement a thin film analyzer (TFA) has been used. We will discuss the influence of temperature effects on the transport properties, including in-situ annealing experiments and the relation to the structure, grain size, and chemical composition which was analyzed with XRD, SEM and EDX.

DS 10.5 Fri 12:15 H1

Passivating polysilicon recombination junctions for crystalline silicon solar cells — •Franz-Josef Haug[1], Audrey Morisset[1], Philippe Wyss[1], Mario Lehmann[1], Aicha Hessler-Wyser[1], Andrea Ingenito[1], Quentin Jeangros[1], Christophe Ballif[1], Shyam Kumar[2], Santhana Eswara[2], and Nathalie Valle[2] — [1]Ecole Poiytechnique Fédérale de Lausanne (EPFL), School of Engineering, PV-Lab, Switzerland — [2]Luxembourg Institute of Science and Technology (LIST), Materials Research and Technology Department, Luxembourg

We investigate polysilicon recombination junctions, whose n-type bottom layer also acts as passivating contact to the silicon surface. They are a key element in tandem devices with a silicon bottom cell, and they could be used to simplify the processing sequence of single-junction cells with interdigitated back contacts. Processing requires high temperatures to crystallize the layers, however, this step can also deteriorate the tunnelling junction by diffusion of dopants. We analyse depth profiles of the doping concentrations in the layers and diffusion across the interface between them by secondary ion mass spectrometry (SIMS) in dynamic mode. We show that undesired diffusion is suppressed by modifying the interface with C, O, or a combination of these. Moreover, we demonstrate that this modification does not interfere with the diffusion of H which is an essential element to passivate defects at the wafer surface. Thus, we find implied open-circuit voltages up to 740 mV for contact resistivities less than 40 mΩcm2, and we demonstrate tandem cells with efficiency above 20%.

DS 10.6 Fri 12:30 H1

Homoepitaxial diamond lateral growth: a new methodology for the next generation of power devices — •Fernando Lloret[1], Daniel Araujo[2], David Eon[3], and Etienne Bustarret[3] — [1]Department of Applied Physics, University of Cádiz, 11510, Puerto Real (Cádiz) Spain — [2]Department of Material Science, University of Cádiz, 11510, Puerto Real (Cádiz) Spain — [3]Univ. Grenoble-Alpes, CNRS, Institut Néel, 38000 Grenoble, France

Diamond is expected to be the base material for future power electronic devices. However, the technological steps and the particularities inherent to the material remain impassable issues for its industrial

implementation. Shortcomings such as the high density of substrate defects and small substrate sizes (less than 1 cm2), the large number of required non-fully-controlled technology steps (etch and deposition or growth) or electrical problems related to the classical geometries (high electric fields, leakages*) can be overcome by using lateral growth. The progress of this promising diamond deposition methodology, capable of drastically reducing defects density, promoting selective doping and providing a wealth of alternative geometries for the device, is here reviewed.

DS 10.7 Fri 12:45 H1

Impact of electrical current on single GaAs nanowire structure — •Ullrich Pietsch[1], Danial Bahrami[1], Ali AlHassan[1], Arman Davtyan[1], Taseer Anjum[1], Ren Zhe[2], Rainer Timm[2], Lutz Geelhaar[3], Jesus Herranz[3], and Dmiri Novikov[4] — [1]University of Siegen, Siegen, Germany — [2]University of Lund, Lund , Sweden — [3]Paul Drude Institute, Berlin, Germany — [4]DESY, Hamburg, Germany

The impact of electrical current on the structure of single free-standing Be-doped GaAs nanowires grown on a Si 111 substrate has been investigated by X-ray nano-diffraction before and after the application of an electrical current. The conductivity measurements of same nanowires in their as-grown geometry have been realized via W-probes installed inside a dual beam focused ion beam/scanning electron microscopy chamber. Comparing reciprocal space maps of the 111 Bragg reflection before and after the conductivity measurement, we find a deformation of the hexagonal nanowire cross-section, tilting and bending with respect to the substrate normal. For electrical current densities above 347 A/mm^2, the diffraction pattern was completely distorted. Confirmed by SEM the reconstructed cross-section of the illuminated nanowire shows elongation of two pairs of opposing side facets accompanied by shrinkage of the third pair of facets. To explain our findings, we suggest material melting due to Joule heating during voltage/current application accompanied by anisotropic deformations induced by the W-probe.

DS 11: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Friday 13:30–14:45 Location: H4

DS 11.1 Fri 13:30 H4

Femtosecond contact-free nanoscopy of ultrafast interlayer transport in 2D heterostructures — •Felix Schiegl[1], Markus Plankl[1], Paulo Eduardo Faria Junior[1], Fabian Mooshammer[1], Tom Siday[1], Martin Zizlsperger[1], Fabian Sandner[1], Simon Maier[1], Markus Andreas Huber[1], Martin Gmitra[1,4], Jaroslav Fabian[1], Jessica Louise Boland[1,2], Tyler Liam Cocker[1,3], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]Photon Science Institute, Department of Electrical and Electronic Engineering, University of Manchester, Manchester, UK — [3]Department of Physics and Astronomy, Michigan State University, East Lansing, MI, USA — [4]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia

Tunneling is one of the most direct results of quantum mechanics, and a hallmark of interlayer exciton formation in semiconducting van der Waals heterostructures. Here, we introduce a new contact-free terahertz nanoscopy technique to trace ultrafast charge dynamics in both conducting and non-conducting materials. We demonstrate $< 50\,\mathrm{nm}$ spatial and subcycle temporal resolution and probe the interlayer tunneling across an atomically sharp WSe_2/WS_2 interface. Pronounced variations of the formation and annihilation of excitons emerge as a direct result of nanoscale strain and changes in atomic registry. Our results show the potential of this technique for revealing how ultrafast tunneling shapes the functionalities of a broad range of condensed matter systems.

DS 11.2 Fri 13:45 H4

Moiré phonons in twisted $MoSe_2$-WSe_2 heterobilayers and their correlation with interlayer excitons — •Philipp Parzefall[1], Johannes Holler[1], Marten Scheuck[1], Andreas Beer[1], Kai-Qiang Lin[1], Bo Peng[2], Bartomeu Monserrat[2,3], Philipp Nagler[1], Michael Kempf[4], Tobias Korn[4], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, UK — [3]Department of Materials Science and Metallurgy, University of Cambridge, UK — [4]Institut für Physik, Universität Rostock, Deutschland

We report about the investigation of twisted $MoSe_2$-WSe_2 heterobilayers by means of low-frequency Raman spectroscopy (LFRS) and low-temperature micro photoluminescence (μPL). We identify moiré phonons of both constituting materials in heterobilayers, which enables us to determine the relative twist angles of the heterobilayers on a local scale with high precision. Atomically reconstructed regions, which are identified by the observation of an interlayer shear mode in LFRS experiments, exhibit in μPL a strong, momentum-allowed interlayer-exciton signal.

DS 11.3 Fri 14:00 H4

Transport Properties of Bulk Black Phosphorus Below and Above the Quantum Limit — •Davide Pizzirani[1], Jasper Linnartz[1], Claudius Müller[1], Brian Kiraly[2], Alexander Khajetoorians[2], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

Black phosphorus (bPh) has emerged as a promising and novel platform for nano-electronic applications due to its in-plane anisotropy and direct band gap that depends on the sample thickness. We present low-temperature magneto-transport experiments on bulk bPh up to 30 T with thicknesses ranging from 40 to 100 μm. A negative magnetoresistance (MR) that turns into a positive linear one is found by increasing the magnetic field. This MR remains quasi-isotropic upon changing the tilt angle from out-of-plane to in-plane with respect to the applied magnetic field. Using samples with different carrier concentrations, we are able to determine the transport properties below and above the quantum limit, and in the regime of variable range hopping.

DS 11.4 Fri 14:15 H4

Excitation-induced optical nonlinearities and charge carrier localization in atomically thin TMD semiconductors — •Daniel Erben, Alexander Steinhoff, Michael Lorke, Christian Carmesin, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen

To interpret the nonlinear optical properties of atomically thin transition metal dichalcogenides (TMD), the density of photoexcited carriers is of central importance. However, in experiments the excited carrier density is practically not accessible. For above band-gap optical pumping of TMD monolayers, we utilize the semiconductor Bloch equations to determine the excitation density as function of the optical pump fluence. Our theory includes Pauli-blocking, band-gap renormalization, dephasing and screening of the Coulomb interaction due to excited carriers. The excitation density strongly depends on the wavelength of the exciting laser pulse. For pumping at the band gap, Pauli blocking of available phase space and renormalizations of the single particle energies are the dominant sources of a nonlinear density dependence, even at small pump fluence. In another study, we investigate the charge-carrier confinement in TMD nanobubbles. These are formed during stacking processes and exhibit quantum light emission upon optical excitation. We demonstrate that the emission originates from strong carrier localization, caused by the interplay of surface wrinkling, strain-induced confinement, and local changes of the dielectric environment. These effects combine to a specific localization signature that is found in recent spatially resolved photoluminescence experiments.

DS 11.5 Fri 14:30 H4

Spatio-temporal dynamics of phonon sidebands in 2D materials — •Roberto Rosati[1], Koloman Wagner[2], Samuel Brem[1], Raül Perea-Causín[3], Jonas D. Ziegler[2], Jonas Zipfel[2], Takashi Taniguchi[4], Kenji Watanabe[4], Alexey Chernikov[2,5], and Ermin Malic[1,3] — [1]Philipps University of Marburg — [2]University of Regensburg — [3]Chalmers University of Technology — [4]National Institute for Materials Science — [5]Dresden University of

Technology

The semiconducting monolayers of transition metal dichalcogenides (TMDs) display a complex manifold of bright and dark exciton states, the latter giving rise to sharp phonon sidebands (PSB) in low-temperature photoluminescence. In this joint theory-experiment study we theoretically predict and experimentally demonstrate time-resolved low-temperature PSB, thus gaining direct access to the evolution of dark excitons in time, energy and space [1,2]. In an excellent theory-experiment agreement we reveal a spectral red-shift of phonon sidebands on a time scale of tens of picoseconds due to phonon-driven thermalization of initially-formed hot momentum-dark excitons [1]. After confined optical excitation, such hot-exciton distribution gives rise to a transient exciton diffusion one order of magnitude faster than the conventional diffusion observed at later times [2]. The obtained insights are applicable to other 2D materials with multiple exciton valleys.

[1] Rosati, R. et al. ACS Photonics 7, 2756 (2020).
[2] Rosati, R. et al. arXiv:2105.10232 (2021).