Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture halls H13, H14, H15, and H17; Poster P1 and P3)

Invited and Prize Talks

HL 3.1	Mon	9:30–10:00	H17	**Alexandria Database - Improving machine-learning models in materials science through large datasets** — •Jonathan Schmidt, Tiago Cerqueira, Aldo Romero, Silvana Botti, Miguel Marques
HL 3.2	Mon	10:00–10:30	H17	**Generative Models on the Rise - Which one shall I pick for my Inverse Design Problem?** — •Hanna Türk, Elisabetta Landini, Christian Kunkel, Patricia König, Christoph Scheurer, Karsten Reuter, Johannes Margraf
HL 3.3	Mon	10:30–11:00	H17	**Machine-learning accelerated prediction of two-dimensional conventional superconductors** — Thalis H. B. da Silva, Théo Cavignac, Tiago F. T. Cerqueira, •Haichen Wang, Miguel A. L. Marques
HL 3.4	Mon	11:15–11:45	H17	**Machine Learning for Design, Understanding, and Discovery of (Semiconducting) Materials** — •Pascal Friederich
HL 3.5	Mon	11:45–12:15	H17	**OptiMate: Artificial intelligence for optical spectra** — •Malte Grunert, Max Grossmann
HL 18.1	Tue	9:30–10:00	H17	**Ultrafast Nano-Spectroscopy of Photo-Induced Dynamics in Low-Dimensional Materials** — •Takashi Kumagai
HL 18.2	Tue	10:00–10:30	H17	**Landau level Nanoscopy of charge and heat transport in low-dimensional heterostructures** — •Mengkun Liu
HL 18.3	Tue	10:30–11:00	H17	**Real space mapping of electrically tunable anisotropic THz plasmon polaritons in hBN encapsulated black phosphorus** — •Eva Pogna
HL 18.4	Tue	11:15–11:45	H17	**Ultra-confined THz hyperbolic phonon polaritons in a transition metal dichalcogenide** — Ryan A. Kowalski, Niclas S. Mueller, Gonzalo Alvarez-Perez, Maximilian Obst, Katja D. Granados, Giulia Carini, Aditha Senarath, Saurabh Dixit, Richarda Niemann, Ragu B. Iyer, Felix Kaps, Jakob Wetzel, J. Michael Klopf, Ivan I. Kravchenko, Deliang Bao, Sokrates T. Pantelides, Martin Wolf, Lukas Eng, Pablo Alonso-Gonzalez, Susanne Kehr, Thomas G. Folland, •Alexander Paarmann, Joshua D. Caldwell
HL 18.5	Tue	11:45–12:15	H17	**Programmable polariton nanophotonics using phase-change materials** — •Thomas Taubner
HL 30.1	Wed	9:30–10:00	H13	**Exploring semiconducting epigraphene grown by polymer-assisted sublimation growth** — •Teresa Tschirner, Julia Guse, Stefan Wundrack, Frank Hohls, Klaus Pierz, Hans Werner Schumacher
HL 30.2	Wed	10:00–10:30	H13	**Huge Enhancement of the Giant Negative Magnetoresistance with Decreasing Electron Density** — •Lina Bockhorn, Christian Reichl, Werner Wegscheider, Rolf J. Haug
HL 30.3	Wed	10:30–11:00	H13	**Ultrafast quantum optics with single-photon emitters in 2D materials** — •Steffen Michaelis de Vasconcellos
HL 30.4	Wed	11:15–11:45	H13	**Realistic simulation of quantum emitter dynamics made easy** — •Moritz Cygorek
HL 30.5	Wed	11:45–12:15	H13	**Data-driven Design of Next Generation 2D Materials and Their Heterostructures** — •Rico Friedrich

HL 34.1	Wed	9:30–10:00	H17	**From complex internal dynamics to emission characteristics control in quantum billiards** — •Martina Hentschel
HL 34.2	Wed	10:00–10:30	H17	**Positioning of microcavities around single emitters** — •Tobias Huber-Loyola
HL 34.3	Wed	10:30–11:00	H17	**Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities** — •Jan Wiersig
HL 34.4	Wed	11:15–11:45	H17	**Correlations and statistics in cavity embedded quantum dot sources of quantum light** — •Ana Predojevic
HL 34.5	Wed	11:45–12:15	H17	**Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum** — •Dario Ballarini
HL 42.1	Wed	16:45–17:15	H17	**Quantum key distribution with single photons from quantum dots** — Joscha Hanel, •Jingzhong Yang, Jipeng Wang, Vincent Rehlinger, Zenghui Jiang, Frederik Benthin, Tom Fandrich, Jialiang Wang, Fabian Klingmann, Raphael Joos, Stephanie Bauer, Sascha Kolatschek, Ali Hreibi, Eddy. Patrick Rugeramigabo, Michael Jetter, Simone. Luca Portalupi, Michael Zopf, Peter Michler, Stefan Kueck, Fei Ding
HL 46.1	Thu	9:30–10:00	H15	**Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System** — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, Manfred Bayer
HL 46.6	Thu	11:15–11:45	H15	**Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules** — •Annika Janssen
HL 47.1	Thu	9:30–10:00	H17	**Quantum-Dot Quantum Light Sources in Deployed Systems** — •Peter Michler
HL 47.2	Thu	10:00–10:30	H17	**Field test of semiconductor quantum light sources** — •Fei Ding
HL 47.3	Thu	10:30–11:00	H17	**Quantum dot based quantum communication in urban networks** — •Rinaldo Trotta
HL 47.4	Thu	11:15–11:45	H17	**Quantum communication protocols over a 14-km urban fiber link** — •Jürgen Eschner
HL 60.1	Fri	9:30–10:00	H17	**Constructing Artificial Matter in the Electron Microscope - Atomic Fabrication at Scale in CrSBr** — •Julian Klein
HL 60.2	Fri	10:00–10:30	H17	**Tuning the structure and magnetism in CrSBr via external pressure** — •Ece Uykur
HL 60.3	Fri	10:30–11:00	H17	**A theoretical perspective on exciton-magnon coupling and its implications** — •Akashdeep Kamra
HL 60.4	Fri	11:15–11:45	H17	**Exciton and valley properties of monolayer transition metal dichalcogenides on the van der Waals magnetic semiconductor CrSBr** — •Yara Galvao Gobato
HL 60.8	Fri	12:30–13:00	H17	**Electric field control of intra- and interlayer excitons in CrSBr** — •Nathan Wilson, Amine Ben Mhenni, Ferdinand Menzel, Alain Dijkstra, Zdenek Sofer, Jonathan Finley

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff, Matthias Florian, Frank Jahnke
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger, Julian Wiercinski, Moritz Cygorek

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

HL 1.1–1.13	Mon	9:30–13:00	H13	**Perovskite and Photovoltaics I (joint session HL/KFM)**
HL 2.1–2.13	Mon	9:30–13:00	H15	**2D Semiconductors and van der Waals Heterostructures I**
HL 3.1–3.8	Mon	9:30–13:00	H17	**Focus Session: Machine Learning of semiconductor properties and spectra**
HL 4.1–4.10	Mon	15:00–17:45	H3	**2D Materials and their Heterostructures I (joint session DS/HL)**
HL 5.1–5.12	Mon	15:00–18:00	H11	**2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
HL 6.1–6.14	Mon	15:00–18:45	H13	**Materials and Devices for Quantum Technology I**
HL 7.1–7.3	Mon	15:00–15:45	H14	**Semiconductor Lasers**
HL 8.1–8.5	Mon	15:00–16:15	H15	**2D Semiconductors and van der Waals Heterostructures II**
HL 9.1–9.6	Mon	15:00–16:30	H17	**Oxide Semiconductors I**
HL 10.1–10.9	Mon	15:00–17:15	H19	**Spin-Dependent Phenomena in 2D (joint session MA/HL)**
HL 11.1–11.10	Mon	16:00–18:45	H14	**Ultra-fast Phenomena I**

HL 12.1–12.6	Mon	16:45–18:15	H15	**Quantum Transport and Quantum Hall Effects (joint session HL/TT)**
HL 13.1–13.7	Mon	16:45–18:30	H17	**Heterostructures, Interfaces and Surfaces**
HL 14.1–14.11	Tue	9:30–13:00	H3	**2D Materials and their Heterostructures II (joint session DS/HL)**
HL 15.1–15.6	Tue	9:30–11:00	H13	**Quantum Dots and Wires: Growth and Properties**
HL 16.1–16.9	Tue	9:30–12:00	H14	**Organic Semiconductors**
HL 17.1–17.13	Tue	9:30–13:00	H15	**2D Semiconductors and van der Waals Heterostructures III**
HL 18.1–18.8	Tue	9:30–13:00	H17	**Focus Session: Nanoscale Light-matter Interaction I**
HL 19.1–19.9	Tue	9:30–13:15	H36	**Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)**
HL 20.1–20.25	Tue	10:00–12:30	P3	**Poster I**
HL 21.1–21.7	Tue	10:30–12:15	H6	**Graphene: Electronic Structure and Excitations (joint session O/HL)**
HL 22.1–22.10	Tue	10:30–13:00	H8	**2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)**
HL 23.1–23.7	Tue	11:15–13:00	H13	**Quantum Dots and Wires: Transport (joint session HL/TT)**
HL 24.1–24.3	Tue	12:15–13:00	H14	**Thermal Properties**
HL 25.1–25.8	Tue	13:30–15:30	P3	**Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)**
HL 26.1–26.5	Tue	13:30–15:30	P3	**Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
HL 27.1–27.5	Tue	13:30–15:30	P3	**Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)**
HL 28.1–28.5	Tue	14:00–15:15	H16	**Topological Insulators (joint session MA/HL)**
HL 29.1–29.96	Tue	18:00–20:00	P1	**Poster II**
HL 30.1–30.5	Wed	9:30–12:15	H13	**Focus Session: Young Semiconductor Forum**
HL 31.1–31.10	Wed	12:15–13:00	H13	**Focus Session: Young Semiconductor Forum Poster**
HL 32.1–32.6	Wed	9:30–11:00	H15	**Nitrides: Preparation and Characterization I**
HL 33.1–33.7	Wed	11:15–13:00	H15	**Nitrides: Devices**
HL 34.1–34.5	Wed	9:30–12:15	H17	**Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)**
HL 35.1–35.8	Wed	10:30–12:45	H11	**2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)**
HL 36.1–36.11	Wed	15:00–18:00	H13	**Materials and Devices for Quantum Technology II**
HL 37.1–37.2	Wed	15:00–15:30	H15	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)**
HL 38.1–38.3	Wed	15:00–15:45	H17	**Nanomechanical systems (joint session HL/TT)**
HL 39.1–39.25	Wed	15:00–18:00	P3	**Poster III**
HL 40.1–40.13	Wed	15:30–19:00	H15	**2D Semiconductors and van der Waals Heterostructures IV**
HL 41.1–41.3	Wed	15:45–16:30	H17	**Spin Phenomena in Semiconductors**
HL 42.1–42.6	Wed	16:45–18:30	H17	**Quantum Dots and Wires: Optics I**
HL 43.1–43.6	Wed	17:00–18:30	H31	**Twisted Materials / Systems (joint session TT/HL)**
HL 44.1–44.3	Wed	18:00–18:45	H13	**Focus Session: Quantum Technologies in Deployed Systems I**
HL 45.1–45.13	Thu	9:30–13:00	H13	**Perovskite and Photovoltaics II (joint session HL/KFM)**
HL 46.1–46.11	Thu	9:30–13:00	H15	**Optical Properties**
HL 47.1–47.7	Thu	9:30–12:30	H17	**Focus Session: Quantum Technologies in Deployed Systems II**
HL 48.1–48.7	Thu	9:30–12:45	H36	**Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)**
HL 49.1–49.8	Thu	10:30–12:30	H11	**2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)**
HL 50.1–50.11	Thu	15:00–17:45	H6	**2D Materials: Stacking and Heterostructures (joint session O/HL)**
HL 51.1–51.8	Thu	15:00–17:15	H13	**Transport Properties (joint session HL/TT)**
HL 52.1–52.8	Thu	15:00–17:15	H14	**Oxide Semiconductors II**
HL 53.1–53.8	Thu	15:00–17:15	H15	**2D Semiconductors and van der Waals Heterostructures V**
HL 54.1–54.8	Thu	15:00–17:15	H17	**Ultra-fast Phenomena II**
HL 55.1–55.13	Thu	15:00–18:30	H33	**Graphene and 2D Materials (joint session TT/HL)**
HL 56	Thu	17:30–19:00	H17	**Members' Assembly**
HL 57.1–57.13	Fri	9:30–13:00	H13	**Quantum Dots and Wires: Optics II**
HL 58.1–58.4	Fri	9:30–10:30	H14	**Nitrides: Preparation and Characterization II**
HL 59.1–59.8	Fri	9:30–11:45	H15	**2D Semiconductors and van der Waals Heterostructures VI**

HL 60.1–60.8	Fri	9:30–13:00	H17	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)**
HL 61.1–61.4	Fri	10:45–11:45	H14	**THz and MIR physics in semiconductors**
HL 62.1–62.5	Fri	11:45–13:00	H15	**2D Semiconductors and van der Waals Heterostructures VII**
HL 63.1–63.5	Fri	12:00–13:15	H14	**Focus Session: Nanoscale Light-matter Interaction II**

Members' Assembly of the Semiconductor Physics Division

Thursday 17:30–19:00 H17

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2026
- Verschiedenes

HL 1: Perovskite and Photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00 Location: H13

HL 1.1 Mon 9:30 H13

Oxygen-Mediated (0D) Cs4PbX6 Formation during Open-Air Thermal Processing Improves Inorganic Perovskite Solar Cell Performance — Rafikul Ali Saha[1], •Wei-Hsun Chiu[2], Giedrius Degutis[1], Peng Chen[3], Matthias Filez[4], Eduardo Solano[5], Nikolai Orlov[6], Francesco De Angelis[7], Carlo Meneghini[7], Christophe Detavernier[4], Sawanta S. Mali[8], Minh Tam Hoang[2], Yang Yang[2], Erik C. Garnett[9], Lianzhou Wang[3], Hongxia Wang[2], Maarten B. J. Roeffaers[1], and Julian A. Steele[3] — [1]KU Leuven, Belgium — [2]Queensland University of Technology, Brisbane, Australia — [3]The University of Queensland, Brisbane, Australia — [4]Ghent University, Belgium — [5]ALBA synchrotron, Barcelona, Spain — [6]AMOLF, Amsterdam, The Netherlands — [7]Roma Tre University, Rome, Italy — [8]Chonnam National University, Gwangju, South Korea — [9]University of Amsterdam, The Netherlands

We highlight the beneficial role of ambient oxygen during the open-air thermal processing of metastable γ-CsPbI3-based perovskite thin films and devices. Physiochemical-sensitive probes elucidate oxygen intercalation and the formation of Pb-O bonds in the perovskite, entering via iodine vacancies at the surface, creating superoxide (O2-) through electron transfer reactions, which drives the formation of a zero-dimensional (0D) Cs4PbI6 protective capping layer during annealing (>330°C). Applied to γ-CsPbI2Br perovskite solar cells, it boosts the operational stability and photo-conversion efficiency of champion devices from 12.7% to 15.4% when annealed in dry air.

HL 1.2 Mon 9:45 H13

Compositional Engineering of Mixed-Metal Chalcohalides for Photovoltaic Applications — •Pascal Henkel[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, P.O.Box 11100, 00076 AALTO, Finland — [2]School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China — [3]Technical University of Munich, 85748 Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaic's [1], that could overcome the stability and toxicity problems of halid perovskites [2], and still deliver high conversion efficiencies [3]. Compositional engineering enables the optimization of MMCH materials properties en route to commercialization.

We study the stability of MMCH alloys for three different compositional positions: the M(III), the Ch and the X site. We use a combination of density functional theory and machine learning to explore the compositional space of the alloys [4] and to compute their convex hulls. For x site alloying, for example $[Sn_2InS_2(Br_{1-c}I_c)_3]$, we obtained stable structures for $c = \frac{1}{3}$ and $c = \frac{2}{3}$ for the *Cmcm* phase and for $c = \frac{1}{6}$ and $c = \frac{1}{3}$ for the $Cmc2_1$ phase, but not for $P2_1/c$. The energetically favored structures (at $c = \frac{1}{3}$) are highly symmetrical and exhibit a layered pattern. Every third halogen layer is fully occupied by iodine whereas the other two layers are filled with bromine.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Z. Anorg. Allg. Chem.* **468**, 91-98 (1980), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Phys. Rev. Materials* **6**, 113801 (2024).

HL 1.3 Mon 10:00 H13

Versatile Two-Step Process for Enhanced Stability and Efficiency in Perovskite Top Cells for Tandem Photovoltaics — •Ronja Pappenberger[1,2], Roja Singh[1,2], Alexander Diercks[2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany

To achieve highly efficient 2T perovskite/silicon (Si) tandem solar cells (TSCs), textured-front Si bottom cells provide superior light-harvesting capabilities, making higher short-circuit current densities of TSC possible. A promising approach to fabricating uniform, high-quality perovskite films on these textured Si cells is the solution-based two-step method. One of the main challenges for perovskite solar cells (PSCs) remains their long-term stability. While methylammonium (MA)-based PSCs have demonstrated some of the highest efficiencies, their instability continues to pose a major obstacle. In this work, a versatile two-step process is employed – replacing MA with formamidinium – which maintains high efficiency, improves open-circuit voltage and enhances stability. A further performance boost is achieved by implementing a dual passivation strategy using $PDAI_2$ and BAI for bulk and surface passivation. This leads to a stable power output exceeding 20.8% for $E_g = 1.67$ eV due to reduced non-radiative recombination at the perovskite/ETL interface and improved film crystallization, enhancing charge carrier extraction. The long-term stability is also distinctly improved. When implemented on textured Si bottom cells, this process delivers efficiencies exceeding 24% for lab-scale monolithic perovskite/Si TSCs with a 1 cm^2 active area.

HL 1.4 Mon 10:15 H13

Recombination at grain boundaries in Cd(Te,Se) thin films in comparison with other photovoltaic absorber layers — •Luka Blazevic[1], Sebastian Weitz[1], Elisa Artegiani[2], Alessandro Romeo[2], and Daniel Abou-Ras[1] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Universita di Verona, Italy

The role of grain boundaries on the device performance is of concern for all polycrystalline absorbers in photovoltaic solar cells. In the present work, recombination velocities s_{GB} at grain boundaries in Cd(Te,Se) thin-film absorbers were determined from cathodoluminescence (CL) intensity distributions, which were acquired together with electron backscatter diffraction (EBSD) and energy-dispersive X-ray spectroscopy (EDXS) maps. The resulting s_{GB} values exhibited ranges over several orders of magnitude ($10^1 - 10^3$ cm/s). These wide value ranges are in good agreement with those obtained on other photovoltaic absorber materials (multicrystalline Si, $Cu(In,Ga)Se_2$, $Cu_2ZnSn(S,Se)_4$). The present work suggests a model comprising the enhanced, nonradiative Shockley-Read-Hall recombination at grain boundaries as well as the upward/downward band bending (± several 10 meV) at these planar defects. This model can reproduce successfully the experimental s_{GB} values from various photovoltaic absorber materials and provides also ranges for the effective defect densities as well as their capture cross-sections at the grain boundaries. It will be shown that typical losses in the open-circuit voltage of the corresponding solar cells due to grain-boundary recombination in the absorbers are few 10 mV.

HL 1.5 Mon 10:30 H13

Microscopic origins of band-gap broadening and its relationship with Urbach tails in photovoltaic absorbers — •Daniel Abou-Ras — Helmholtz-Zentrum Berlin, Germany

The broadening of absorption edges is a general feature found in numerous semiconductors used as absorber layers for thin-film solar cells. Since this broadening gives rise to radiative losses of the open-circuit voltage, it is of importance to control the broadening by corresponding material design of the photovoltaic absorber materials. The present work provides an overview of the microscopic origins of band-gap broadening, addressing not only compositional aspects and microstrain, but also electrical and optoelectronic properties on the sub-μm scale. In addition, the Urbach energy extracted from absorptance or quantum efficiency spectra has been used broadly to quantify disorder in a material. However, up to date, it has not only not been clarified what the microscopic origins of Urbach tails are; the present contribution also shows that there is no direct correlation between the broadening of the absorption edge and the Urbach energy of a semiconductor, as verified for about 30 different photovoltaic absorbers.

HL 1.6 Mon 10:45 H13

Minimizing V_{OC} losses in high bandgap perovskite solar cells for the application in perovskite/perovskite/silicon triple-junction solar cells — •Athira Shaji[1,2], Minasadat Heydarian[1,3], Oliver Fischer[1,3], Michael Günthel[1], Orestis Karalis[4], Maryamsadat Heydarian[1], Alexander J. Bett[1], Hannes Hempel[4], Martin Bivour[1], Florian Schindler[1], Martin C. Schubert[1], Stefan W. Glunz[1,3], Andreas W. Bett[1,2], Juliane Borchert[1,3], and Patricia S. C. Schulze[1] — [1]Fraunhofer Institute for Solar Energy Systems ISE, Germany — [2]University Freiburg, Institute of Physics, Germany — [3]University of Freiburg, Department of Sustainable Systems Engineering, Germany — [4]Helmholtz-Zentrum Berlin, Solar Energy Division, Germany

The high bandgap (HBG) top cell is the main source of V_{OC} loss in perovskite/perovskite/silicon triple junction solar cells due to photoinduced phase segregation, non-radiative recombination at the per-

ovskite bulk and interface with the charge transport layers (CTLs), as well as energetic misalignment between the perovskite layer and the CTLs. The starting point of this work was a triple-cation double-halide perovskite composition with a bandgap of 1.83 eV. By implementing a multi-faceted optimization approach, an average improvement in V_{OC} of 250 mV was achieved for HBG perovskite solar cells. Replacing the reference HBG perovskite with the optimised top cell in perovskite/perovskite/silicon triple-junction solar cells results in the improvement of V_{OC} by 124 mV, and the champion device achieves a voltage above 3 V.

15 min. break

HL 1.7 Mon 11:15 H13

The Effect of Overdamped Phonons on the Fundamental Band Gap of Perovskites — •Xiangzhou Zhu and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Different from conventional semiconductors, halide perovskites (HaPs) exhibit unique anharmonic fluctuations that strongly influence optoelectronic properties. Recent studies have shown that in specific temperature regimes, the strong phonon-phonon interactions in HaPs lead to overdamped phonons, where vibrational lifetimes drop below one oscillation period. However, the relationship between these overdamped phonons and atomic fluctuations, as well as their impact on optoelectronic properties, are not fully understood. Here, using molecular dynamics (MD) simulations and augmented stochastic Monte Carlo methods that account for phonon renormalization and imaginary modes, we contrast the band gap behavior of two anharmonic perovskite materials, $SrTiO_3$ and $CsPbBr_3$, of which only the latter exhibits overdamped phonons.[1] Our results show that the overdamped phonon dynamics in $CsPbBr_3$ drive slow atomic fluctuations that are not adequately captured by conventional phonon quasiparticle descriptions. Importantly, we show that these overdamped phonon lead to significant renormalization of the band gap. Our work disentangles the consequences of anharmonic effects on the optoelectronic properties and electron-phonon interactions in perovskites.

[1] Zhu, X. & Egger, D. A. arXiv:2406.05201 (2024).

HL 1.8 Mon 11:30 H13

Polymorphism at surface in $CsPbI_3$ from first principles — •Jasurbek Gulomov[1], Guido Roma[1], Jacky Even[2], and Marios Zacharias[2] — [1]Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif sur Yvette, 91191, France — [2]Université Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

Halide perovskites show great potential for optoelectronics and photovoltaics, but challenges with ion migration and phase stability remain.Atomic-scale phenomena at surfaces and interfaces must be understood to block ion migration and enhance passivation. A peculiar property of these materials is the tendency to gain energy by disordered structural distortions, dubbed polymorphism, in contrast to the view of a perfectly symmetric monomorphous structure. Using first-principles calculations, we investigate the electronic and structural properties of polymorphous bulk $CsPbI_3$ and its 100 surface with two terminations. For the bulk, we generate a dynamically stable polymorphous structure for the cubic high-temperature phase using the method recently proposed by M. Zacharias et al. [1]. The energy gain and band gap opening are essentially linked to the increased average length of Pb-I bonds. Then we extend the concept of polymorphism to the surface, analyzing surface dipoles and work functions by comparing monomorphous and polymorphous slabs with experimental data. Our results tend to confirm the occurrence of polymorphism at surfaces in $CsPbI_3$.

[1] Zacharias, M., et al., npj Comput. Mater. 9, 153 (2023).

HL 1.9 Mon 11:45 H13

Benchmarking approximations for the theoretical prediction of positron lifetimes in halide perovskites — Kajal Madaan[1], •Guido Roma[1], Jasurbek Gulomov[1], Pascal Pochet[2], Catherine Corbel[3], and Ilja Makkonen[4] — [1]Université Paris-Saclay, CEA, Service de recherches en Corrosion et Comportement des Matériaux, SRMP, 91191 Gif sur Yvette, France — [2]Department of Physics, IriG, Univ. Grenoble-Alpes and CEA, Grenoble, France — [3]LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, 91120, France — [4]Department of Physics, University of Helsinki, P.O. Box 43, FI-00014 Helsinki, Finland

Positron annihilation spectroscopy is a well recognized tool for probing vacancies in materials. Recent applications of this technique to $APbX_3$ halide perovskites are sparse, and the rare theoretical predictions of positron lifetimes in these materials, published in association with experiments, do not fully agree with each other. These works suggest that vacancies on the A site are not detected. In our theoretical study we thoroughly revisit and compare several approximations for the electron-positron correlation functional, applied to methylammonium lead iodide ($MAPbI_3$) and $CsPbI_3$ and their vacancies. The discrepancies between the approaches make it difficult to unequivocally exclude the presence of methylammonium vacancies in $MAPbI_3$. Moreover, when using a truly nonlocal electron-positron correlation functional, the predicted positron density in a vacancy presents peculiar features and a much lower binding energy to the vacancy with respect to semilocal approximations.

HL 1.10 Mon 12:00 H13

Dynamics of electronic surface states in halide perovskites using machine-learning force fields — •Frederico Delgado[1], Frederico Simões[1], Waldemar Kaiser[1], Leeor Kronik[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The photovoltaic performance exhibited by bulk halide perovskites (HaPs) hinges on their excellent optoelectronic properties, which have been extensively investigated. Nonetheless, extended defects like surfaces are ubiquitous, and as such, their impact on such properties requires further, careful investigation. Rigorous examination of dynamics in this context through ab-initio molecular dynamics implies large computational costs, which are here circumvented by the use of machine learning (ML) force fields. In this study, we demonstrate the transient and shallow nature of surface states in $CsPbBr_3$. We shed light on the mechanisms which underpin the behaviour of such states through the framework of local, internal dipoles. Our results aid in rationalizing the benign nature of surfaces in $CsPbBr_3$, and further the understanding of the correlation between structural dynamics and optoelectronic properties of HaP surfaces.

HL 1.11 Mon 12:15 H13

Comprehensive High-Throughput DFT Study of Intrinsic Defects and Dopability in p-type Zn3P2 for Photovoltaic Applications — •Nico Kawashima[1,2,3] and Silvana Botti[1,3] — [1]Ruhr-Universität, Bochum, Germany — [2]Friedrich-Schiller-Universität, Jena, Germany — [3]RC FEMS, Bochum, Germany

Zn_3P_2 has attracted significant interest as a thin-film absorber material for photovoltaic applications due to its intrinsic p-type conductivity and earth-abundant constituents. However, the nature of the dominant native defects – whether phosphorus interstitials (P_i) or zinc vacancies (V_{Zn}) – remains a subject of debate, with implications for the material's electronic structure and dopability through mechanisms such as Fermi-level pinning and defect compensation.

We perform a high-throughput density functional theory (DFT) analysis to systematically investigate both intrinsic point defects and potential extrinsic dopants. By resolving the ground-state configurations and formation energies of key native defects, we provide a clearer understanding of their impact on the electronic landscape. This insight is then applied to evaluate a range of extrinsic dopants, predicting their incorporation and activation potentials in the presence of native defects.

Our study offers a comprehensive framework that links intrinsic defect behavior with extrinsic doping strategies, providing critical guidance for tuning the electrical properties of Zn_3P_2. The findings present experimentally actionable insights that can drive the optimization of Zn_3P_2 for next-generation photovoltaic devices.

HL 1.12 Mon 12:30 H13

Density functional theory study of hydrogen passivation mechanisms in defective silicon — •Hania Azzam[1], Tobias Binninger[1], and Michael Eikerling[1,2] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Silicon heterojunction (SHJ) solar cells offer high-effeciency energy conversion, with reported efficiencies up to 27%. Their performance

and durability depend on effective passivation of dangling bonds at the amorphous/crystalline silicon interface, where electron-hole recombination reduces efficiency. Hydrogen atoms play a crucial role in passivating those dangling bonds, minimizing recombination loses. Recent experimental studies by IMD-3 at Forschugnszentrum Jülich showed performance improvements after light soaking, a process where solar cells are exposed to intensive light at elevated temperatures. It is hypothesized that light soaking activates hydrogen migration toward defect sites. This theoretical study explores hydrogen passivation mechanisms in defective silicon for SHJ solar cells. Using Density Functional Theory (DFT), we analyze how silicon vacancies alter the electronic structure of Si-H systems, introducing localized defect states within the band gap and shifts in Fermi level, and subsequently investigate the changes induced by hydrogen passivation. These insights contribute to understanding the beneficial effects of light soaking on SHJ solar cells.

HL 1.13 Mon 12:45 H13

First principles theory of nonlinear long-range electron-phonon interaction — •Matthew Houtput[1,2], Luigi Ranalli[2], Jacques Tempere[1], and Cesare Franchini[2] — [1]University of Antwerp, Belgium — [2]University of Vienna, Austria

Electron-phonon interactions in a solid are crucial for understanding many interesting material properties, such as transport properties and the temperature dependence of the electronic band gap. For harmonic materials, the linear interaction process where one electron interacts with one phonon is sufficient to quantitatively describe these properties. However, this is no longer true in anharmonic materials with significant electron-phonon interaction, such as quantum paraelectrics and halide perovskites. Currently, the only available models for nonlinear electron-phonon interaction are model Hamiltonians, written in terms of phenomenological parameters. Here, we provide a microscopic semi-analytical expression for the long-range part of the 1-electron-2-phonon matrix element, which can be interfaced with first principles techniques. We show that unlike for the long-range 1-electron-1-phonon interaction, the continuum approximation is not sufficient and that the entire phonon dispersion must be taken into account. We calculate an expression for the quasiparticle energies and show that they can be written in terms of a 1-electron-2-phonon spectral function. To demonstrate the method in practice, we calculate the 1-electron-2-phonon spectral function for $KTaO_3$ from first principles. The framework in this article bridges the gap between model Hamiltonians and first-principles calculations for the 1-electron-2-phonon interaction.

HL 2: 2D Semiconductors and van der Waals Heterostructures I

The session covers the photonic properties and corresponding devices made from 2D semiconductors and van der Waals heterostructures.

Time: Monday 9:30–13:00 Location: H15

HL 2.1 Mon 9:30 H15

Probing strong electron-phonon coupling in graphene by resonance Raman spectroscopy with infrared excitation energy — •Simone Sotgiu[1,2], Tommaso Venanzi[1], Lorenzo Graziotto[1], Francesco Macheda[1], Taoufiq Ouaj[2], Elena Stellino[1], Bernd Beschoten[2], Christoph Stampfer[2], Francesco Mauri[1], and Leonetta Baldassarre[1] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

Resonance Raman spectroscopy (RRS) has been a key asset to study the interplay between electronic and vibrational properties of graphene. We report on RRS measurements with an excitation photon energy down to 1.17 eV on mono (MLG) and bilayer (BLG) graphene, to study how low-energy carriers interact with lattice vibrations. Thanks to the excitation energy close to the Dirac point, we unveil in the MLG a giant increase of the intensity ratio between the double-resonant 2D and 2D* Raman peaks with respect to graphite [1]. In BLG, the low excitation energy hampers some of the resonant Raman processes giving rise to the 2D peak. Consequently, the subfeatures composing the 2D mode are spectrally more separated with respect to visible excitations. We compare experimental measurements on BLG with ab initio theoretical calculations and we trace back such modifications on the joint effects of probing the electronic dispersion close to the band splitting and enhancement of electron-phonon matrix elements [2]. [1] T. Venanzi et al., Phys. Rev. Lett. 2023, 130, 256901 [2] L. Graziotto et al., Nano Lett. 2024, 24, 1867

HL 2.2 Mon 9:45 H15

Nonlinear Probing of Ultrafast Bandgap Modulations in Atomically Thin Semiconductors — •Sebastian Klimmer[1,2], Thomas Lettau[3], Jan Wilhelm[4,5], Dragomir Neshev[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]ARC Centre of Excellence for Transformative Meta-Optical Systems, Department of Electronic Materials Engineering, Research School of Physics, The Australian National University, Canberra, Australia — [3]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Jena, Germany — [4]Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [5]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany

Bandgap modulations are pivotal for semiconductor based applications, typically achieved by permanent modifications of material composition or size. Recently, dynamic, ultrafast bandgap modulations have been demonstrated in transition metal dichalcogenides, exploiting the valley exclusive optical Stark (OS) and Bloch-Siegert (BS) shifts. However, their detection requires state of the art two-color pump-probe schemes. Here, we show a simplified method by measuring the second-harmonic (SH) power dependence in monolayer WSe_2. The fundamental beam (FB) blue-shifts the bandgap by OS/BS shifts, which scale linearly with intensity, resulting in a enhanced (reduced) SH signal, depending on the detuning $E_g - 2\hbar\omega_{FB}$. Our experimental data are fully explained by an analytical SBE model, which allows us to extract values for the transition dipole element and dephasing time.

HL 2.3 Mon 10:00 H15

Detecting out-of-plane polarized luminescence in TMDs with laser-written waveguide circuits — •Alina Schubert[1], Karo Becker[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Matthias Heinrich[1], and Tobias Korn[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]2Ferdinand Braun Institut, Leibnitz Institut für Höchstfrequenztechnik, Berlin, Germany

Photoluminescence (PL) spectroscopy is used widely to investigate the outstanding excitonic properties of two-dimensional crystals. However, since these measurements are typically performed in vertical incidence, the sample is excited with light polarized in the plane of its layer. Despite, these detection schemes systematically neglect the out-of-plane polarized components of the emitted signal that propagate along the layer and therefore are only accessible by side-on detection.

Here, a side-on detection is achieved by using femtosecond laser direct written waveguides in fused silica glass as substrates [1]. By inscribing the waveguides directly under the surface of the glass, interactions of the waveguide's evanescent field and the sample are enabled in a controlled fashion. Therefore, the sample can be excited due to its proximity to the waveguide, while, in turn, the excitonic emission can be coupled into the waveguide and subsequently be detected.

In this work, the in-plane propagating luminescence in TMDs is analyzed with a particular focus on determining influences on the signal resulting from combining TMDs and surface waveguides.

[1] A. Szameit et al., J. Phys. B.: At. Mol. Opt. Phys., 43 (2010).

HL 2.4 Mon 10:15 H15

Current-induced second-harmonic generation in monolayer graphene-devices — •Nele Tornow[1], Friederike Renz-Wieland[1], Omid Ghaebi[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

In pristine and isolated graphene, second-order nonlinear optical processes are, within the dipole approximation, forbidden due to the invariance under space inversion symmetry. Few studies have suggested

that inversion symmetry can be broken by in-plane currents, leading to a measurable second-harmonic generation (SHG) [1,2]. In particular, investigations have shown that interfacial charge trapping between a monolayer graphene and silicon dioxide (SiO_2) on silicon substrate results in electrically tunable SHG when driving in-plane currents [2]. To further verify this hypothesis, we study current-tunable second-harmonic emission in two graphene based devices: one high-quality double-encapsulated hexagonal boron nitride/graphene field-effect transistor and one with a graphene-SiO_2 interface, finding SHG only in the latter one.

Our findings provide insights into the origin of current-tunable SHG and the mechanisms underlying space inversion symmetry breaking in graphene.

[1] Dean, J. et al., Appl. Phys. Lett. 26, 261910 (2009)
[2] An, Y. et al., Nano Lett. 13, 2104-2109 (2013)

HL 2.5 Mon 10:30 H15

Electron-phonon coupling across the TMD/hBN van der Waals interface — •Gianmarco Gatti[1,2], Christophe Berthod[3], Julia Issing[2], Michael Straub[2], Salony Mandloi[2], Yann Alexaniann[2], Anna Tamai[2], and Felix Baumberger[2] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland — [3]Department of Theoretical Physics, University of Geneva, Geneva, Switzerland

The lattice mismatch at van der Waals interfaces is widely used to engineer single particle band structures supporting complex quantum phases in two dimensions. Electronic states in van der Waals heterostructures may also couple to bosonic excitations in an adjacent substrate. These interfacial interactions are difficult to identify, and it is commonly assumed that they play a marginal role. Here, we reveal that quasiparticles in monolayer transition metal dichalcogenides (TMDs) are dressed by a remote cloud of phonons in the adjacent hexagonal boron nitride slab. Using angle resolved photoemission, we identify replica bands in the TMDs which are a clear fingerprint of a long-range electron-phonon interaction. We develop a modified Fröhlich model that shows quantitative agreement with the experimental spectral functions and discuss the properties of this model. Our analysis shows that remote electron-phonon coupling is a generic property of interfaces with hBN. This has implications for electron mobilities in 2D materials, for superconductivity and possibly for moiré correlated phases.

HL 2.6 Mon 10:45 H15

Polaron spectroscopy of many-body systems — •Ivan Amelio — Université Libre de Bruxelles, Brussels, Belgium

When an impurity is immersed in a many-body background, it is dressed by the excitations of the bath, and forms "a polaron".

As a result, the injection spectrum of the impurity carries the hallmarks of the correlations present in the bath. This physics is relevant for excitons optically injected in a few layer heterostructure, or for cold atomic mixtures.

In this talk, we will first review the basic theoretical framework and recent experimental progress.

Then, we will theoretically analyze a few cases of correlated many-body states: the impurity injection spectra are predicted to display peculiar features, that allow to distinguish whether the bath features BCS pairing, charge density waves, topological phases, the BKT transition, etc.

15 min. break

HL 2.7 Mon 11:15 H15

Ultrafast All-Optical Probe of Broken Time-Reversal Symmetry in Monolayer WSe_2 — •Paul Herrmann[1], Sebastian Klimmer[1], Thomas Lettau[1], Till Weickhardt[1], Anastasios Papavasileiou[2], Kseniia Mosina[2], Zdeněk Sofer[2], Jan Wilhelm[3], and Giancarlo Soavi[1] — [1]Friedrich Schiller University Jena, Germany — [2]University of Chemistry and Technology, Prague, Czech Republic — [3]University of Regensburg, Germany

The combination of broken space inversion and preserved time-reversal symmetry (TRS) underlies the spin-valley degree of freedom in monolayer transition metal dichalcogenides (TMDs). Introduction of an imbalance between the energy degenerate, but non-equivalent valleys (local extrema of the bandstructure) at the ±K points of the Brillouin zone breaks TRS. We probe broken TRS and a valley imbalance on ultrashort time scales by comparing the second harmonic (SH) intensity for a circularly *vs.* linearly polarized fundamental beam (FB). By numerically and analytically solving the semiconductor Bloch equations, we show that a two-photon resonant right/left circularly polarized FB interacts exclusively with the ±K valley. Thus, a circularly polarized FB probes the C_{3h} wave vector group of the ±K valleys, in contrast to a linearly polarized FB probing the D_{3h} group of the Γ point. This difference between wave vector groups at K and Γ fully captures and explains the experimentally measured deviation from the otherwise expected ratio of 2 in the circular *vs.* linear SH intensities.

HL 2.8 Mon 11:30 H15

Layer number sensitive Raman modes of atomically thin layered MoS_2 — •Henry Hübschmann[1], Gerhard Berth[1], Klaus Jöns[1], Katharina Burgholzer[2], and Alberta Bonanni[2] — [1]PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany — [2]Johannes Kepler University Linz, Linz, Austria

The material group of TMDCs like molybdenum disulfide has gained great attention in the fields of quantum technologies over the last decade due to their particular electronic and optical properties [1]. 2D-MoS_2 has found many applications in optoelectronics and photonics, where the tunable electronic band gap exhibiting strong strutural dependency is an essential feature [2]. Here Raman spectroscopy represents the method of choice for the layer number identification of such 2D structures [3].

This work deals with layer structure sensitive phonon modes of mechanically exfoliated 2D-MoS_2 utilizing Raman analysis. Regarding the two main phonon modes occuring we successfully observed corresponding Raman shifts for monolayer to nine-layer configurations showing a specific dependency on the layer number, enabling the unambiguous determination of the layer number. Besides the two dominant vibrations many other phonon modes are identified, assigned to the symmetry and analyzed in the same manner. Within our comprehensive study we found other structure sensitive phonon modes, showing specific dependency on the layer number, expanding the set of Raman modes for the investigation of 2D-MoS_2 and its properties.

HL 2.9 Mon 11:45 H15

Universal and ultrafast probe of broken time-reversal symmetry — •Florentine Friedrich[1], Paul Herrmann[1], Sebastian Klimmer[1], Zdeněk Sofer[2], Shridhar Sanjay Shanbhag[3], Jan Wilhelm[3], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [3]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Germany

Time-reversal symmetry (TRS) defines some of the most fundamental properties of condensed matter, such as the relation between energy, spin and Berry curvature, therefore influencing features like topology or non-trivial spin textures. Two-dimensional transition metal dichalcogenides (TMDs) offer the possibility to engineer TRS and space-inversion symmetry independently, rendering them excellent model systems. TRS in TMDs can be lifted *via*, *e.g.* valley-selective bandgap opening. Nonlinear optics (NLO) as a probe of TRS is non-invasive and ultrafast; however, detection *via* second harmonic generation is limited to non-centrosymmetric systems. In this work, we make the nonlinear all-optical probe of broken TRS universal by utilizing polarization-resolved third harmonic generation (THG), which is always present also in centro-symmetric crystals. As a proof of principle, we probe broken TRS in a TMD monolayer, by using elliptically polarized light, leading to valley and spin asymmetric gap opening. We then test our method on a TMD bilayer, probing broken TRS in a centrosymmetric system with THG for the first time.

HL 2.10 Mon 12:00 H15

Ultrafast pump-probe spectroscopy of WSe_2 multilayer bubbles — •Jens-Christian Drawer, Henri Melchert, Marti Struve, Christian Schneider, and Martin Esmann — Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Heterostructures of van der Waals materials have recently emerged as a versatile platform for the tailored generation and detection of coherent acoustic phonons in the GHz up to THz frequency range [1]. In this work, we investigate WSe_2 layers of different thicknesses by ultrafast pump-probe spectroscopy and observe thickness-dependent breathing-type acoustic phonon modes up to 850 GHz in frequency in the bilayer case. Under suitably chosen conditions for the dry-gel stamping prepa-

ration, 40 nm thick WSe_2 flakes form nanobubbles. For these bubbles, our pump-probe measurements reveal a significant improvement in the quality factor of their fundamental 29 GHz acoustic Fabry-Pérot mode from $Q = 13.9 \pm 0.7$ to $Q = 141 \pm 5$. We then tailor these high-Q modes by encapsulating the bubbles with hBN, introducing new spectral features attributed to coupled acoustic modes between WSe_2 and hBN. For example, our approach may enable the ultrafast modulation of strain-defined quantum emitters found in WSe_2.

[1] Yoon, Y. et al.. Nature 631, 771–776 (2024).

HL 2.11 Mon 12:15 H15

Polarized optical contrast spectroscopy of in-plane anisotropic van-der-Waals heterostructures — Ernst Knöckl[1,2], •Alexandre Bernard[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany

To properly exploit interfacial symmetry breakings in van der Waals (vdW) heterostructures, giving rise to emergent behaviors, it is crucial to determine the symmetry axes of the individual layers.

I will discuss polarized optical contrast spectroscopy as a simple and non-destructive approach to characterize the crystalline anisotropy and orientation of 2D materials in vdW heterostructures. We developed a 3D-printed motorized polarization module compatible with typical microscope platforms, allowing broadband polarization-resolved reflectance spectroscopy. We investigated the in-plane birefringence of exfoliated MoO3 thin films (optically transparent) and few-layer WTe2 crystals (semi-metallic). We compared the measured spectra to a model based on a transfer matrix formalism.

Contrasting with other polarization-sensitive approaches, such as Raman or second harmonic generation spectroscopy, this method requires orders of magnitude less excitation power densities, avoiding degradation of delicate layers. Furthermore, it allows quick and simple polarization-sensitive absorbance measurements to resolve anisotropic excitonic properties in symmetry-breaking heterostructures or anisotropic semiconductors.

HL 2.12 Mon 12:30 H15

Microscopic comparison of TMD and QW laser capabilities — •Tommy Schulz, Daniel Erben, Alexander Steinhoff, and Frank Jahnke — Institut für theoretische Physik, Bremen, Germany

The lasing capabilities of monolayer transition metal dichalcogenides (TMDs) are compared to quantum wells (QWs). For material-realistic calculations of the optical gain we connect tight-binding bandstructures for TMDs and $\vec{k} \cdot \vec{p}$ band structures for QWs and the respective interaction matrix elements with state of the art many-body theory. The semiconductor Bloch equations are solved for highly excited materials, where Coulomb interaction is treated selfconsistently on a GW level together with carrier-phonon interaction. While TMDs provide larger material gain, they also exhibit large shifts of the peak gain with increasing high excitation densitiy, thereby limiting the lasing capabilities.

HL 2.13 Mon 12:45 H15

Strong coupling between light confined in a dielectric nanocavity and excitons in a monolayer TMDC — •Frederik Schröder[1,2], Paweł Wyborski[1], Meng Xiong[1,2], George Kountouris[1,2], Battulga Munkhbat[1], Martijn Wubs[1,2], Philip T. Kristensen[1,2], Jesper Mørk[1,2], and Nicolas Stenger[1,2] — [1]Department of Electrical and Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]NanoPhoton - Center for Nanophotonics, Technical University of Denmark, Ørsteds Plads 345A, DK-2800 Kgs. Lyngby, Denmark

Enhancing light-matter interactions with optical nanocavities is essential for many applications, such as nanolasers and quantum technologies. Recently, advances in the design and fabrication of extreme dielectric confinement (EDC) cavities enabled the confinement of electromagnetic fields in InP on the tens of nanometer scale without being limited by absorption losses [1]. We demonstrate experimentally strong light-matter interactions between excitons in a single layer of $MoTe_2$ and light confined in an EDC nanocavity. The avoided crossing of the system is verified with both photoluminescence and reflection measurements. The observed Rabi-energy of 10.1 meV exceeds the averaged losses in the system [2]. These results pave the way for future studies on nonlinearities at the single-photon level [3].

[1] M. Xiong et al., *Opt. Mater. Express*, 14, 397 (2023), [2] F. Schröder et al., *in preparation*, [3] E. V. Denning et al., *Phys. Rev. Res.*, 4, L012020 (2022)

HL 3: Focus Session: Machine Learning of semiconductor properties and spectra

The focus session highlights recent advances of machine learning concepts for the characterization of semiconductors. It particularly spotlights ML-driven advances in the prediction of key semiconductor properties, such as band gaps, dielectric constants and optical spectra, which are critical for the design of next-generation energy materials.

The focus session is organized by Erich Runge (TU Ilmenau).

Time: Monday 9:30–13:00 Location: H17

Invited Talk HL 3.1 Mon 9:30 H17

Alexandria Database - Improving machine-learning models in materials science through large datasets — •Jonathan Schmidt[1], Tiago Cerqueira[3], Aldo Romero[4], Silvana Botti[2], and Miguel Marques[2] — [1]Department of Materials, ETH Zürich, Zürich, CH-8093, Switzerland — [2]Research Center Future Energy Materials and Systems of the University Alliance Ruhr and ICAMS, Ruhr University Bochum, D-44801, Bochum, Germany — [3]CFisUC, Department of Physics, University of Coimbra, Coimbra, PortugalLarga, 3004- — [4]Department of Physics, West Virginia University, Morgantown, WV, 26506, USA

Accurate machine learning models hinge on the availability of large, high-quality datasets for both training and validation - a need that is particularly acute in materials science due to the scarcity of robust datasets. To address this gap, we present Alexandria, an open-access database generated through high-throughput studies using crystal-graph-attention networks to identify novel, stable crystal structures. The database includes over five million density-functional theory calculations for periodic compounds spanning one, two, and three dimensions.

Leveraging data generated with higher fidelity exchange-correlation functionals, we also explore the effectiveness of transfer learning strategies in detail. Finally, we assess to what extent incorporating experimental data can further enhance predictions of DFT band gaps.

Schmidt, Jonathan, et al. Materials Today Physics 48 (2024): 101560.

Invited Talk HL 3.2 Mon 10:00 H17

Generative Models on the Rise - Which one shall I pick for my Inverse Design Problem? — •Hanna Türk[1,2], Elisabetta Landini[2], Christian Kunkel[2], Patricia König[2], Christoph Scheurer[2], Karsten Reuter[2], and Johannes Margraf[2,3] — [1]EPFL, Lausanne, Switzerland — [2]Fritz-Haber-Institut der MPG, Berlin, Germany — [3]Universität Bayreuth, Bayreuth, Germany

The pursuit of novel materials through computational discovery appears endless due to the vast space of potential structures and compositions. For inorganic materials, this complexity is heightened by the combinatorial possibilities presented by the periodic table, where even a single-crystal structure can theoretically exhibit millions of compositions.

Recently, generative machine learning models have emerged as method for direct exploration of the material design space. Here, we evaluate the efficacy of various conditioned deep generative models, including reinforcement learning, variational autoencoders, and generative adversarial networks, in the prototypical task of designing Elpasolite compositions with low formation energies. Utilizing the fully

enumerated space of 2 million main-group Elpasolites, we rigorously assess the precision, coverage, and diversity of the generated materials. Furthermore, we develop a hyperparameter selection scheme tailored for generative models in chemical composition space. Finally, we demonstrate the power of these machine learning models on a realistic application.

[1] Chem. Mater. 2022, 34, 9455-9467.

Invited Talk HL 3.3 Mon 10:30 H17

Machine-learning accelerated prediction of two-dimensional conventional superconductors — Thalis H. B. da Silva[2], Théo Cavignac[1], Tiago F. T. Cerqueira[2], •Haichen Wang[1], and Miguel A. L. Marques[1] — [1]Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstraße 150, D-44801 Bochum, Germany — [2]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal

We perform a large-scale search for two-dimensional (2D) superconductors, by using electron-phonon calculations with density-functional perturbation theory combined with machine learning models. In total, we screened over 140 000 2D compounds from the Alexandria database. Our high-throughput approach revealed a multitude of 2D superconductors with diverse chemistries and crystal structures. Moreover, we find that 2D materials generally exhibit stronger electron-phonon coupling than their 3D counterparts, although their average phonon frequencies are lower, leading to an overall lower T_c. In spite of this, we discovered several out-of-distribution materials with relatively high-T_c. In total, 105 2D systems were found with $T_c > 5$ K. Some interesting compounds, such as CuH_2, NbN, and V_2NS_2, demonstrate high T_c values and good thermodynamic stability, making them strong candidates for experimental synthesis and practical applications. Our findings highlight the critical role of computational databases and machine learning in accelerating the discovery of novel superconductors.

15 min. break

Invited Talk HL 3.4 Mon 11:15 H17

Machine Learning for Design, Understanding, and Discovery of (Semiconducting) Materials — •Pascal Friederich — Karlsruher Institut für Technologie

Machine learning can accelerate the screening, design and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on graph neural networks for property prediction [1] and understanding of structure-property relations [2], as well as on the use of machine learning for automated data analysis and autonomous decision-making in self-driving labs, especially in the area of semiconductor optimization for photovoltaics [3,4].

[1] Reiser et al., Communications Materials 3 (1) (2022), https://www.nature.com/articles/s43246-022-00315-6

[2] Teufel et al., xAI (2023), https://arxiv.org/abs/2211.13236

[3] Wu et al., JACS 2023, https://pubs.acs.org/doi/full/10.1021/jacs.3c03271

[4] Wu et al., Science 2024

Invited Talk HL 3.5 Mon 11:45 H17

OptiMate: Artificial intelligence for optical spectra — •Malte Grunert and Max Grossmann — Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Machine Learning (ML) is currently transforming computational materials science - many material properties can now be predicted to *ab initio* accuracy almost instantly using modern ML techniques. Until recently, optical properties such as absorption in the UV/VIS region were excluded from the ever-growing list of machine-learned properties, due to lack of high-quality training data for electronic excitations. To address this missed opportunity, we present OptiMate [1], a graph attention neural network trained on the largest high-quality, high-throughput dataset of optical properties available to date – a dataset that we have independently generated. OptiMate is capable of predicting the complex optical properties of a wide class of materials up to the XUV range with quantitative accuracy. In addition, OptiMate learns physical properties of spectra like continuity and causality directly from high-quality data, without such properties being enforced by constraints in the model architecture or with penalties during training. We detail the workings of OptiMate, show that it (and probably other complex models) learns a surprisingly meaningful representation of the material space, and preview current developments such as transfer learning to higher levels of theory.

[1] M. Grunert *et al.*, Phys. Rev. Mater. **8**, L122201 (2024)

HL 3.6 Mon 12:15 H17

Mechanical Properties of Hybrid Perovskites study using explainable Machine Learning — •Yuxuan Yao[1,2], Dan Han[3], and Harald Oberhofer[2] — [1]Chair for Theoretical Chemistry, Technical University of Munich — [2]Chair for Theoretical Physics VII, University of Bayreuth — [3]School of Materials Science and Engineering, Jilin University

Lead-based halide perovskite photovoltaics are of great interest for use in optoelectronic devices due to the high power conversion efficiency and low cost. 2D hybrid organic and inorganic perovskites (HOIPs) have been utilized as capping layers on top of 3D perovskites to increase the stability. On top of that, soft and stable HOIPs are an attractive material for use in flexible electronic devices. We utilize explainable machine learning (ML) techniques to accelerate the in silico prediction of elasticities of 2D perovskites, based on their Young's moduli. Our ML models allow us to distinguish between stiff and nonstiff HOIPs and to extract the materials' features most strongly influencing their elasticities. The Pb-halogen-Pb bond angle and the cations' steric effect indices (STEI) emerge as the dominant physical feature with an inverse correlation to the structural non-stiffness. The deformation of the octahedra strongly affects the material's mechanical properties, which allows us to perform the transferability test from single-layered to multi-layered 2D perovskites. Overall, our work thus points the way towards future design efforts of HOIPs with regards to their elasticity.

HL 3.7 Mon 12:30 H17

Exploring Strongly Anharmonic Thermal Insulators with Machine-Learned Interatomic Potential using an Active Learning Scheme — •Shuo Zhao, Kisung Kang, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max Planck Society

Thermal insulating semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as defect creation and phase-transition precursors [1]. These phenomena disrupt the conventional phonon picture and render perturbative methods ineffective or even incorrect for describing heat transport, leading to a substantial challenge for reliable prediction of thermal conductivity. This work presents a framework that combines the Green-Kubo formalism with machine-learned interatomic potentials, enhanced by a sequential active learning scheme [2]. Equivariant neural networks `NequIP` [3] and `So3krates` [4] are employed and systematically compared for this purpose. Based on this framework, we examine 15 materials that possibly have ultra-low thermal conductivity previously, predicted by a symbolic regression machine-learning model [5]. Our demonstrations and results not only provide precise thermal conductivity predictions for strongly anharmonic systems but also pave the way for accelerated exploration and design of novel thermal insulators.

[1] F. Knoop, *et al.*, *Phys. Rev. Lett.* **130**, 236301 (2023). [2] K. Kang, *et al.*, arXiv:2409.11808 (2024). [3] S. Batzner, *et al.*, *Nat. Commun.* **13**, 2453 (2022). [4] J.T. Frank, *et al.*, *Nat. Commun.* **15**, 6539 (2024). [5] T.A.R. Purcell, *et al.*, *Npj Comput. Mater.* **9**, 112 (2023).

HL 3.8 Mon 12:45 H17

Learning an effective Hamiltonian for large-scale electronic-structure calculations — •Martin Schwade and David A. Egger — TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale systems across various temperatures using conventional density functional theory (DFT) often encounters significant computational challenges. Recent advancements in machine learning force fields (ML-FFs) have made it easier to generate atomic trajectories at different temperatures. However, determining the electronic structure with temperature dependence remains a difficult task. Building on our earlier work involving a temperature-transferable tight-binding (TB) model [1] to learn an effective Hamiltonian, we introduce an extension of this method that leverages machine learning techniques to increase the accuracy and transferability of this approach. By integrating ML with TB mod-

els, this strategy offers a promising pathway to evaluate temperature-dependent material properties with reduced computational demands.

[1] M. Schwade, M.J. Schilcher C. Reverón Baecker, M. Grumet, D. A. Egger, J. Chem. Phys. 160, 134102 (2024)

HL 4: 2D Materials and their Heterostructures I (joint session DS/HL)

Time: Monday 15:00–17:45 Location: H3

HL 4.1 Mon 15:00 H3

Nanoscale NMR of two-dimensional solids using NV centers in diamond — •Marcel Martin[1], Mokessh Kannah Ciwan[1], Yejin Lee[2], Jakob Nachtigal[1], Nicola Poccia[3,4], Uri Vool[2], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [4]Department of Physics, University of Naples Federico II, Naples, Italy

Nuclear magnetic resonance (NMR) is a powerful method to investigate electronic properties of condensed matter but is inherently limited by its low sensitivity. Nitrogen-vacancy (NV) centers in diamond are quantum sensors that allow extending NMR to thin films and μm-scale exfoliated flakes of 2D materials which exhibit electronic phases such as charge density waves (CDW) and superconductivity. For the latter, NMR is especially powerful as it can elucidate the pairing symmetry of the charge carriers.
In this talk, we first discuss solid-state nano-NMR with NV centers of CaF_2, a testbed material for this method. The ultimate goal, however, is to study the CDW and Ising superconductivity phases of few-layer NbSe2 with nano-NMR. In this context, we present initial optical studies of $NbSe_2$ flakes which have been exfoliated and transferred onto a diamond. In addition to this, we will present results of conventional NMR on bulk $NbSe_2$ which serve as a reference.

HL 4.2 Mon 15:15 H3

Twist-tunable spin control in twisted bilayer bismuthene — •Ludovica Zullo[1,2,3,4], Domenico Ninno[4,5], and Giovanni Cantele[5] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France — [4]Dipartimento di Fisica E. Pancini, Università degli Studi di Napoli *Federico II*, Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy — [5]CNR-SPIN, c/o Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy

The role of spin-orbit coupling (SOC) in twisted bilayers has gained increasing attention due to its potential for spintronics, opening a quest for new layers with substantial SOC. In this work [1], by means of first principles calculations, we investigate how the interplay between SOC and twist angle impacts the band structure and spin textures of twisted bilayer bismuthene. We find that the twist angle can be deemed a control knob to switch from a small-gap semiconductor to a metallic behavior. Most crucially, the accurate analysis of the energy bands close to Fermi energy reveals a twist-tunable splitting in the mexican-hat shape of the bands that can otherwise be obtained only by applying enormous electric fields, providing insight into innovative technologies for future spintronic devices. [1] Ludovica Zullo, Domenico Ninno, Giovanni Cantele, Phys. Rev. B, 110, 165411 (2024)

HL 4.3 Mon 15:30 H3

Iron Diffusion in Thermally Stable $Ti_3C_2Cl_2$ MXenes under UHV Conditions — •Moritz Vanselow[1], Maksim Riabov[2], Hanna Pazniak[2], Thierry Ouisse[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

MXenes are 2D materials derived from a MAX phase precursor. Molten salt etching of $Ti_3C_2Cl_2$ results in hydrophobic $Ti_3C_2T_X$ MXenes with T_X = -Cl as a termination species [1]. $Ti_3C_2Cl_2$ MXenes are deposited on $Si(100)/SiO_2$ and we in situ study its chemical stability by mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum. Compared with standard hydrophilic $Ti_3C_2T_X$ MXenes, where T_X = -F, =O, and -OH, fluorine and hydroxyl groups can be removed by annealing at temperatures up to 1000 K, the thermal stability of $Ti_3C_2Cl_2$ MXenes is significantly enhanced. Moreover, intercalated water changing the MXene sheet separation, is not present in hydrophobic $Ti_3C_2Cl_2$ as proven by ex situ X-ray diffraction, wide-angle X-ray scattering (WAXS) and X-ray photoelectron spectroscopy (XPS). After optimizing the annealing procedure, we in situ intercalate Fe by e-beam assisted deposition on top of MXene thin films and subsequent Fe diffusion by soft annealing at 600 K. This work is funded by a joint ANR-DFG-Project under ANR-23-CE09-0031-01 and DFG ID 530103526. [1] T. Zhang et al., Chem. Mater. 36, 1998 (2024).

HL 4.4 Mon 15:45 H3

Interactions Between Two-Dimensional Crystals and Molecules via Density Functional Theory — •Stefan Wolff[1], Xin Chen[2], Tobias Dierke[1], and Janina Maultzsch[1] — [1]Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

The unique properties of two-dimensional (2D) materials can be modified through chemical functionalization, driven by their interactions with functional groups or molecules. Density functional theory (DFT) calculations are employed to investigate non-covalent functionalization of bilayer graphene with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) molecules. The interactions between the graphene layers and the HATCN molecules play a significant role in determining the functionalization behavior, which depends on the stacking arrangement. Locally stacked regions within the moiré lattice of twisted bilayer graphene (tBLG) play a crucial role for functionalization. Consequently, the moiré pattern of tBLG can serve as a template to control the degree of functionalization. Furthermore, laser-triggered covalent functionalization of molybdenum disulfide (MoS_2) enables the fabrication of patterned 2D heterostructures with phenyl-based interface linkers. Through DFT calculations, various potential binding motifs and their associated optical properties are predicted. Calculations of reaction energies and Raman modes provide insights into the likelihood of different reaction pathways and the structures they yield.

HL 4.5 Mon 16:00 H3

Toward high-sensitivity and low-power consumption gas sensor devices based on 2D-transistors. — •Aurelio García Valenzuela[1], Zahra Fekri[1], Madhuri Chennur[1], Nikol Lambeva[1], Jens Zscharschuch[1], Victoria Constance Köst[2], Krysztof Nieweglowski[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Electronic Packaging Technology, AVT, TU-Dresden, Germany

Two-dimensional (2D) materials exhibit excellent properties compared to their bulk counterparts and are promising for applications like gas sensors. Their high surface-to-volume ratio and surface-active sites enhance gas absorption and sensitivity, addressing challenges in detecting low concentrations and reducing power consumption.

This work presents the fabrication and testing of 2D materials-based field-effect transistor (FET) gas sensors. Mechanically exfoliated 2D materials are stacked into heterostructures to create back-gated FETs, with device patterning achieved via electron beam lithography.

The devices were exposed to NH3 and NO2 gases at various temperatures. Gas interactions caused systematic changes in p- and n-type currents and shifts in the transfer curve, depending on gas concentration and type (donor or acceptor). These results demonstrate the suitability of 2D materials-based FETs as efficient and sensitive gas sensors.

short break

HL 4.6 Mon 16:30 H3

Pressure-dependent Effective Hamiltonian and Topological Transitions for Twisted Bilayer Transition Metal Dichalcogenides — •Miftah Hadi Syahputra Anfa[1], Sabri Elatresh[1,2],

Hocine Bahlouli[1,3], and Michael Vogl[1,2] — [1]Physics Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia — [2]Interdisciplinary Research Center (IRC) for Intelligent Secure Systems, KFUPM, Dhahran, Saudi Arabia — [3]Interdisciplinary Research Center (IRC) for Advanced Materials, KFUPM, Dhahran, Saudi Arabia

Recent studies have shown the existence of nontrivial topological moire bands in twisted bilayer transition metal dichalcogenides (TMDs), which depend on the twist angle. Motivated by this, we present a study of such a system under applied vertical pressure. The study begins by first considering the untwisted bilayer case without pressure. We find that the system can be described by an effective low-energy Hamiltonian that behaves approximately quadratic and includes layer-shift dependent terms that we were able to determine by symmetry. The structure is then relaxed under pressure in the 0.0 - 3.5 GPa range using ab initio density functional theory (DFT). The DFT band structures for each corresponding pressure are fitted to the effective Hamiltonian to obtain the pressure-dependent parameters. Consecutively, the explicit expression for the twisted pressure-dependent Hamiltonian is obtained by treating the twist as a position-dependent shift between layers. We then present changes in Chern number results for the important energy bands due to pressure.

HL 4.7 Mon 16:45 H3

Effect of spin-dependent tunneling in a $MoSe_2/Cr_2Ge_2Te_6$ van der Waals heterostructure on exciton and trion emission — •Annika Bergmann[1], Swarup Deb[1,2], Veronika Schneidt[1], Mustafa Hemaid[1], Kenji Watanabe[3], Takashi Taniguchi[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, Rostock University, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]Research Center for Electronic and Optical Materials, Tsukuba, Japan — [4]Research Center for Materials Nanoarchitectonics, Tsukuba, Japan

In recent years, thin films of magnetic van der Waals materials have gained increasing interest due to their potential applications in spintronics. For instance, heterostructures (HS) consisting of ferromagnetic CRI_3 and a WSe_2 monolayer have demonstrated the existence of magnetic proximity effects, manifesting in the lifting of WSe_2 valley degeneracy as well as helicity-dependent photoluminescence (PL) emission of the WSe_2 monolayer in proximity to the 2D ferromagnet [1,2]. Here, we study HS consisting of monolayer $MoSe_2$ and few-layer ferromagnetic $Cr_2Ge_2Te_6$ (CGT). Under circularly polarized excitation, PL measurements show that the $MoSe_2$ exciton-trion emission ratio depends on the relative orientation of excitation helicity and CGT magnetization, even though the PL emission itself is unpolarized. This hints at an ultrafast, spin-dependent interlayer charge transfer that competes with exciton and trion formation and recombination.

[1] D. Zhong et al., Science Advances, 3 (2017)
[2] D. Zhong et al., Nat. Nanotechnol. 15 (2020)

HL 4.8 Mon 17:00 H3

Magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Tauqir Shinwari[1], Kacho I. A. Khan[1], Jens Herfort[1], Michael Hanke[1], Chen Chen[2], Joan M. Redwing[2], Achim Trampert[1], Mehak Loyal[3], Gerhard Jakob[3], Mathias Kläui[3], Roman Engel-Herbert[1], and João Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]2D Crystal Consortium Materials Innovation Platform, Materials Research Institute, The Pennsylvania State University, PA, United States — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

Van der Waals (vdW) heterostructures consisting of two-dimensional (2D) ferromagnetic and nonmagnetic materials hold great promises for tailoring their magnetic and transport properties. Here we report on the magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2$ (FGT, with x ≈ 0.2)/WSe_2 heterostructures tailored via the FGT thickness. Magnetic characterizations and anomalous Hall effect measurements with both out-of-plane and in-plane magnetic fields reveal an enhanced perpendicular magnetic anisotropy (PMA) in thinner FGT and a ferromagnetic order up to room temperature. The pronounced unconventional Hall effect (UHE) suggests the possible formation of skyrmions. The thickness-dependent asymmetric magnetoresistance reveals a unique magnetization switching process. Our results demonstrate the high potential of all-epitaxial FGT/WSe_2 heterostructures for the advancement of future 2D spintronic applications.

HL 4.9 Mon 17:15 H3

Effect of Ni-doping on the structural/magnetic properties of large area epitaxial 2D-ferromganet Fe_3GeTe_2 — •Kacho Imtiyaz Ali Khan[1], Tauqir Shinwari[1], Hua Lv[1], Frans Munnik[2], Jens Herfort[1], Michael Hanke[1], and Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Helmholtz-Zentrum Dresden- Rossendorf e.V. Dresden, Germany

2D ferromagnets with strong perpendicular magnetic anisotropy exhibit magnetic order down to the monolayer thickness and have the potential to overcome long-term challenges faced by 3D ferromagnets to build up advanced energy-efficient spintronic devices. In this work, we show the large-area epitaxial growth of Ni-doped Fe_3GeTe_2 films via molecular beam epitaxy. X-ray diffraction measurements demonstrate high-quality epitaxy of pure Fe_3GeTe_2 phase on graphene/SiC(0001) substrates. Magneto-transport measurement unveils the ferromagnetic nature of the film, with strong perpendicular magnetic anisotropy for pure Fe_3GeTe_2 and Ni-doped films. However, the Ni-doped Fe_3GeTe_2 shows a decrease in Curie temperature T_C with an increase in Ni-doping. We believe that the Ni doping modifies the lattice parameters and structure (e.g., Ni intercalation), which results in the dilution of magnetic properties of Fe_3GeTe_2 by reducing the T_C down to 50 K. Our findings show the role of Ni incorporation on the ferromagnetic behavior of Fe_3GeTe_2 films, which is crucial for the development of future spintronic devices.

HL 4.10 Mon 17:30 H3

The epitaxial growth of Gallium Selenide — Michele Bissolo, Marco Dembecki, Florian Rauscher, Jan Schabesberger, Abhilash Uhle, Jonathan J. Finley, Gregor Koblmüller, and •Eugenio Zallo — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Garching, Germany

Group III-VI post-transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are van der Waals semiconductors with layer-dependent electronic, thermoelectric and optical properties, strong photoresponsivity, and a Caldera type valence band [1]. However, the limited scalability and risk of contamination of the standard mechanical exfoliation technique are detrimental to developing devices at an industrial scale. Here, we demonstrate the molecular beam epitaxy growth of PTMC [2] GaSe on 2-inch sapphire wafers. To study the pristine properties of this air-sensitive material in situ, we perform Raman spectroscopy in a UHV chamber directly connected to the growth chamber. Film composition and morphology are investigated by tuning the growth temperature and group VI/III flux ratio and by correlating them with the known spatial gradients across the whole substrate. The combination of these findings with ex-situ surface morphology characterization allows us to construct the phase diagram and identify the 2D layered region [3]. Perspectives on the growth of PTMC on 2D substrates and the epitaxial registry will be discussed. [1] H. Cai, et al., Appl. Phys. Rev. 6, 041312 (2019).[2] E. Zallo, et al., npj 2D Mater. & Appl. 7, 19 (2023).[3] M. Bissolo, et al., [to be submitted].

HL 5: 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Monday 15:00–18:00 Location: H11

HL 5.1 Mon 15:00 H11

Hexagonal structures of europium oxides on Pd(111) studied with LEED and STM — •Muriel Wegner, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

With an increasing interest in technological applications of oxide materials, also two-dimensional (2D) oxides came into focus. The large flexibility in the variation of the cationic species, including even a combination of different cations, promises a rich variety of properties [1,2]. So far, the center of attention has been on transition metal sesquioxides M_2O_3 of corundum structure.

Here, we expand this field towards lanthanides. We present a combined scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) study of the growth of submonolayer coverages of europium oxide on a Pd(111) surface. Upon annealing the as deposited Eu in oxygen containing environments at temperatures above 800 K, long-range ordered multilayer islands of Eu_2O_3 are obtained. From LEED a $\begin{pmatrix} 8/3 & 4/3 \\ -4/3 & 4/3 \end{pmatrix}$ superstructure on Pd(111) is derived, which corresponds to a hexagonal lattice with a lattice parameter of 6.35 Å. This structure exhibits a large stability range. Only upon annealing to 1175 K in UHV an additional (2×2) superstructure evolves, which is seen as a hexagonal array of pores at a distance of 12.70 Å in STM. By addition of small amounts of Ti atoms, the transformation into planar two-dimensional films is achieved. These mixed-metal oxides form a honeycomb lattice with a lattice parameter of 7.2 Å. In contrast to pristine Eu_2O_3, the Ti containing honeycomb can easily be resolved in STM.

[1] M. Van den Bossche, J. Goniakowski, and C. Noguera, Nanoscale **13**, 19500 (2021)
[2] P. I. Wemhoff, N. Nilius, C. Noguera, and J. Goniakowski, J. Phys. Chem. C **126** (10), 5070 (2022)

HL 5.2 Mon 15:15 H11

Growth of an Fe buckled honeycomb lattice on Be(0001) — Hermann Osterhage[1], Abid H. Khan[2], Karoline Oetker[1], Radek Dao[1], Samaneh Setayandeh[2], Patrick Burr[2], Roland Wiesendanger[1], and •Stefan Krause[1] — [1]University of Hamburg, Germany — [2]University of New South Wales, Sydney, Australia

The Be(0001) surface is considered to be an ideal model system to host a 2D electron gas with pronounced electron-electron and electron-phonon interactions that are decoupled from the bulk [1,2]. In a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study the growth of Fe on a clean Be(0001) surface is investigated on the atomic scale [3]. At low Fe coverage, the nucleation of terraced nanoislands with a disordered surface is observed experimentally with STM. Increasing the Fe coverage results in the growth of extended films exhibiting a well-ordered p(2×2) superstructure. DFT is applied to investigate the growth of Fe on a Be(0001) surface from individual atoms to extended films.

The Fe buckled honeycomb lattice formation on Be(0001), as derived from our study, provides evidence for the realization of a very peculiar non-trivial electronic and magnetic model system. The results will be presented and discussed in terms of their implications for the emergence of novel electronic and magnetic phases resulting from the interactions between the 2D electron gas and the magnetic atoms.

[1] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).
[2] H. Osterhage *et al.*, Phys. Rev. B **103**, 155428 (2021).
[3] H. Osterhage *et al.*, Surf. Sci **752**, 122609 (2025).

HL 5.3 Mon 15:30 H11

Electronic structure and edge states in the 2D Kagome lattice Ta_2S_3 / Au(111) — •Thais Chagas[1], Alessia Bardazzi[1], Samuel M. Vasconcelos[2], Alan C. R. Souza[3], Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Daniel Weber[1], Mario S. C. Mazzoni[3], Michael Rohlfing[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Germany — [2]Institute of Solid State Theory, Universität Münster, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Brazil

Kagome structures are a key model system in quantum physics, representing one of the most geometrically frustrated 2D magnetic lattices. In these systems, magnetic moments condense into a spin liquid phase at low temperatures, leading to intriguing physical phenomena. The characteristic Kagome bands in this lattice consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, in contrast, leads to fermions with infinite effective mass.

In this work, we investigate the 2D Ta_2S_3 Kagome phase on Au(111) using scanning tunneling microscopy (STM). STM images reveal bright island edges as a consequence of an enhanced density of states, indicating the presence of edge states. Additionally, we observe a significant dependence of atomic contrast on tunneling conditions, suggesting a complex electronic band structure near the Fermi level. Furthermore, we analyze the impact of growth parameters on defect formation. Finally, density functional theory (DFT) was employed to study the electronic structure of this material on Au(111), providing deeper insight into its electronic properties and interactions.

HL 5.4 Mon 15:45 H11

Spectroscopic and microscopic study of (car)borane based 2D materials — •Martha Frey[1], Julian Picker[1], Jakub Visnak[2], Christof Neumann[1], Tomas Base[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec-Rez, c.p. 1001, Czech Republic

Boranes are electron-delocalized molecular clusters containing boron and hydrogen. Their electron-deficient bonding and structural diversity as well as their high thermal stability make them attractive for applications ranging from optoelectronics to energy storage. Here we present the fabrication of a novel boron-based, carbon free two-dimensional (2D) material via electron-induced crosslinking of borane-based self-assembled monolayers (SAMs) on silver substrates. The SAMs, crosslinking process and resulting nanomembranes were analyzed using complementary surface-sensitive techniques including X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), low-energy electron diffraction (LEED) and scanning tunneling and electron microscopies (STM, SEM). Furthermore, the results were compared with carborane-based 2D nanomaterials studied previously in our labs. The results demonstrate that properties of the 2D (car)borane nanosheets can be adjusted and tailored by the respective SAM constituents and that these structurally diverse cluster molecules open up new avenues for engineering novel functional 2D materials.

HL 5.5 Mon 16:00 H11

Growth and Structure of Titanium Ditelluride Films on Au(111) — •Andreas Raabgrund, Alexander Wegerich, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Aiming at the MBE growth of transition metal ditelluride (MTe_2) films particularly in the single-layer limit, the formation of and interaction with the interface is of fundamental interest. The growth of a MTe_2 film can be achieved either by the tellurization of the desired metal substrate [1] or by the reactive deposition of Te and the corresponding transition metal M on a suitable substrate [2].

In this contribution we follow the latter approach and investigate both single- and multilayer $TiTe_2$ films on Au(111) by LEED-IV, DFT, and STM. At first glance, LEED suggests a (4×4) superstructure with three $TiTe_2$ on four Au(111) unit cells. STM topography, however, reveals a mismatch of about 1% of the growing film w.r.t. the Au(111) substrate which indicates a relaxed $TiTe_2$ layer. LEED-IV results favor a film in close contact with Au substrate (Te-Au layer distance: ≈ 2.7 Å). By DFT total energy calculations we find that neither Te nor Ti substitution is favored in the topmost Au layer. Continuing the reactive deposition of Ti and Te a multilayer $TiTe_2$ film grows epitaxially as found by LEED-IV with a Pendry R factor of 0.12. Further, we discuss the transferability of this growth recipe to other MTe_2 films on Au(111).

[1] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)
[2] K. Lasek et al., ACS Nano **14**, 8473 (2020)

HL 5.6 Mon 16:15 H11

Growth and Edge Reconstruction of 2D MnI_2 on Ag(111) —

•Daniel Rothhardt[1,2,3], Christopher Penschke[4], Hans Josef Hug[1,2], Regina Hoffmann-Vogel[3], and Amina Kimouche[3] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [4]Institute of Chemistry, University of Potsdam, 14476 Potsdam, Germany

The reduced dimensionality of thin transition metal dihalide films on single-crystal surfaces enables a wide array of magnetic and electronic phenomena. However, producing stoichiometric monolayer islands demands thorough control over growth parameters. In this work, we utilize scanning probe microscopy (SPM) to explore the growth of MnI_2 on Ag(111) through single-crucible evaporation. The Ag(111) surface's catalytic activity promotes dehalogenation of MnI_2, resulting in a reconstructed iodine adlayer that serves as a template for the formation of truncated hexagonal MnI_2 islands. These islands display alter-nating edge lengths and distinctive Kelvin potentials, as revealed by Kelvin Probe Force Microscopy (KPFM). Density Functional Theory (DFT) calculations corroborate the experimental observations, including island heights, lattice parameters, and edge formation energies for both pristine and reconstructed edges. The asymmetry in edge lengths arises from differences in formation energies, determined by the orientation (up or down) of iodine atoms at the edges, as confirmed by DFT.

HL 5.7 Mon 16:30 H11

Low defect density in MoS_2 monolayers grown on Au(111) by metal-organic chemical vapor deposition — •Julian Picker, Ziyang Gan, Christof Neumann, Antony George, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany

Monolayers of transition metal dichalcogenides (TMDs) possess high potential for applications in novel electronic and optoelectronic devices and therefore the development of methods for their scalable growth is of high importance. Among different suggested approaches, metal-organic chemical vapor deposition (MOCVD) is the most promising one for technological applications because of its lower growth temperature compared to most other methods, e.g., conventional chemical vapor or atomic layer deposition (CVD, ALD). Here we demonstrate the epitaxial growth of MoS_2 monolayers on Au(111) by MOCVD at 450 °C. We confirm the high quality of the grown TMD monolayers down to the atomic scale using several complementary methods. These include Raman spectroscopy, non-contact atomic force microscopy (nc-AFM), X-ray photoelectron spectroscopy and scanning tunneling microscopy (STM). The topographic corrugation of the MoS_2 monolayer on Au(111), revealed in a moiré structure, was measured as 20 pm by nc-AFM. The estimated defect density calculated from STM images of the as-grown MoS_2 monolayers is in the order of 10^{12} vacancies/cm^2. The defects are mainly caused by single sulfur vacancies.

J. Picker *et al.*, Micron **186**, 103708 (2024).

HL 5.8 Mon 16:45 H11

Characterization of a large-scale single-domain MoS_2 monolayer — •Fabian Schöttke[1], Luka Pirker[2], Martin Vondráček[3], Michaela Hanušová[2], Václav Valeš[3], Jan Honolka[3], Otakar Frank[2], Matěj Velický[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

To fully utilize the outstanding optical and electronic properties of single-layer transition metal dichalcogenide (TMDC) in devices, a perfect single-domain film is needed. From the wealth of available preparation methods, exfoliation seems to provide the highest film quality. This method, however, commonly results in small flakes within the micrometer regime only. Exfoliation onto, or assisted by, a Au(111) surface is able to result in large-scale single-domain samples of several millimeters in diameter. We experimentally confirm the high quality of a MoS_2 monolayer on Au(111) by characterizing several sample properties: optical appearance, long-range structural order, work function changes, and the occupied & unoccupied electronic structure. Optical inspection and diffraction patterns easily identify millimeter-sized single domains. The electronic structure of MoS_2 is clearly distinguished from Au(111) states, especially measured by inverse photoemission in the L gap of Au(111). In summary, our experimental data of a MoS_2 monolayer exfoliated onto Au(111) demonstrate the capability of this procedure to produce large-scale single-domain TMDC samples.

HL 5.9 Mon 17:00 H11

Kinetics of borophene growth on Ir(111) via boron segregation from the bulk — •Marin Petrović[1], Sherif Kamal[1], Borna Radatović[1], Marko Kralj[1], Matteo Jugovac[2], Iulia Cojocariu[2], Andrea Locatelli[2], and Tevfik Onur Menteş[2] — [1]Centre for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia — [2]Elettra - Sincrotrone Trieste S.C.p.A, 34149 Trieste, Italy

Segregation of boron atoms to the Ir(111) surface and their self-assembly into a borophene monolayer were tracked by low-energy electron microscopy (LEEM). Real-time monitoring of sample temperature, boron adatom concentration and borophene coverage reveals the kinetics of boron segregation from the iridium bulk and different modalities of borophene epitaxial growth. It is found that the temperature-triggered boron segregation to the surface is accompanied by instantaneous nucleation of borophene islands and condensation of boron adatoms, followed by rapid propagation of island perimeter along the iridium terraces. Subsequent growth of borophene proceeds by displacement of iridium surface steps, which is energetically expensive and thus relatively slow process that heavily depends on the step morphology. By identifying and analyzing quasi-equilibrium conditions on the sample surface during borophene growth, formation enthalpy of a boron monomer from borophene was estimated, which agrees well with the available theoretical calculations of the boron-iridium system.

HL 5.10 Mon 17:15 H11

Growth and etching of hBN on Cu(111): Impact on substrate step dynamics and morphology — •Patrick Seleš[1,2], Marin Petrović[1], Smruti Ranjan Mohanty[3], and Frank Meyer zu Heringdorf[3] — [1]Center for Advanced Laser Techniques, Institute of Physics, Bijenička 46, Zagreb, Croatia — [2]Faculty of physics, University of Rijeka, Radmile Matejčić 2, Rijeka, Croatia — [3]Faculty for Physics, University of Duisburg-Essen, Lotharstrasse 1-21, Duisburg, Germany

The interaction of precursors and oxygen molecules with metal surfaces plays an important role in the growth dynamics of two-dimensional material such as graphene and hexagonal boron nitride (hBN). By using low-energy electron microscopy (LEEM), in this study we investigate the influence of hBN growth on Cu(111) step dynamics at various stages ranging from borazine precursor dosing to oxygen etching. Real-time monitoring of Cu step displacement underneath and next to hBN islands revealed step pinning and a significant decrease in step velocities compared to the pristine Cu surface, highlighting the stabilizing effect of hBN. After the removal of hBN islands by oxygen etching, Cu steps accelerated back to the pre-growth velocities and rearranged into a new surface morphology. Our findings elucidate the interplay between surface dynamics and step motion during hBN growth on Cu(111). By analyzing step displacement and morphological evolution, we contribute to a deeper understanding of metal-catalyzed chemical vapor deposition growth of hBN.

HL 5.11 Mon 17:30 H11

In-situ growth and characterization of 2D $TaSe_2$ on Au(111) — •Cathy Sulaiman[1], Lars Buss[1], Raquel Sánchez-Barquilla[1], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany

Group V dichalcogenides such as TaX_2 (X = S, Se, T) have extensively been investigated in recent decades due to their diverse electron correlation effects, including the occurrence of charge density waves and Mott-Hubbard transitions. In 2D, two polytypes, 1T and 1H, exist, which exhibit distinct properties, making selective growth of each polytype crucial. Using low-energy electron microscopy (LEEM), we have successfully observed the growth of two $TaSe_2$ phases on Au(111) *in situ* after the co-deposition of Ta and Se. At elevated temperature, micron-sized, triangle-shaped islands with bright contrast nucleate first and grow at a higher rate. However, this phase turns out to be metastable as it suddenly transitions into a more stable phase (with dark contrast) and continues to grow at a reduced rate. Low-energy electron diffraction shows the presence of $TaSe_2$; bandstructure-sensitive I(V)-LEEM analysis reveals substantial differences in electron reflectivity between both phases. A comparison with TaS_2 suggests that the metastable and stable phases are 1T- and 1H-$TaSe_2$, respectively.

HL 5.12 Mon 17:45 H11

CVD growth of monolayer transition metal dichalcogenides heterostructures using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Julian Picker[1], Christof Neumann[1], Moritz Quincke[2], Johannes Biskupek[2], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena 07743, Germany — [2]Central Facility of Electron Microscopy, Electron Microscopy Group of Material Science, University of Ulm, Ulm 89081, Germany

Heterostructures (HSs) formed of transition metal dichalcogenide (TMD) monolayers have attracted substantial research interest due to their unique physical properties. However, engineering the HS configurations (lateral and vertical) including the domain size for each TMD remains challenging. Here we present a facile route for the synthesis of different types of HSs of TMD monolayers using liquid precursors for transition metals. We characterized the TMD HSs by several complementary spectroscopy and microscopy techniques. Our results suggest that the HS configurations, lateral length and area of each TMD can be tuned by varying concentration ratios of the precursors. In addition, the overall heterostructure sizes can also be tuned from few to hundreds of micrometers. The developed method paves the way to obtaining high-quality lateral and vertical HS of $MoSe_2$-WSe_2 with controllable domain sizes.

HL 6: Materials and Devices for Quantum Technology I

Time: Monday 15:00–18:45 Location: H13

HL 6.1 Mon 15:00 H13

First-Principles Investigation of NV Centers in Silicon Carbide Polytypes — •Timur Biktagirov, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Optically addressable spin defects in semiconductors offer versatile platforms for quantum applications, including computing, communication, and sensing. Among these, nitrogen-vacancy (NV) centers in silicon carbide (SiC) polytypes have emerged as a promising class of quantum defects, analogous to the NV center in diamond. In contrast to diamond, SiC is a technologically mature material with large-scale production capabilities, advanced doping techniques, and compatibility with CMOS fabrication methods. Additionally, the emission wavelengths of NV centers in SiC lie in the near-infrared range, making them particularly suitable for applications in single-photon emission. In this work, we discuss recent advancements in the ab initio investigation of NV centers in the 4H, 6H, and 3C polytypes of SiC. Simulating the magneto-optical properties of these spin centers, which are crucial for quantum applications, requires a detailed and accurate description of both the host material and the embedded defect. Accordingly, we demonstrate how supercell density functional theory (DFT) and recent implementations based on DFT can be employed to model key properties, including intra-defect optical transition energies, electron-electron and electron-nuclear spin interactions, and electron-phonon coupling. These theoretical insights provide a foundation for optimizing NV centers in SiC for next-generation quantum technologies.

HL 6.2 Mon 15:15 H13

tunable superconductivity in Ga-doped SixGe1-x via ion implantation and flash lamp annealing — •yu cheng[1,2], yi li[1,2], oliver steuer[1], mao wang[3], artur erbe[1,2], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Laboratory of Micro-Nano Optics, College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu, PR China

Group-IV superconducting semiconductors offer promising opportunities for scalable superconductor-semiconductor platforms in quantum computing. However, realizing a superconducting phase in semiconductors requires doping concentrations beyond the metal-insulator transition (MIT). Achieving such high doping levels in silicon (Si) and germanium (Ge) is challenging due to the limited solid solubility of acceptors in these materials. Various advanced techniques have been developed to overcome this problem, such as gas immersion laser doping or ns-pulsed laser melting [1]. Here, we explore tunable superconducting states in Ga-hyperdoped SixGe1-x alloys by applying ion implantation followed by ms-range flash lamp annealing. We observed that the critical temperature depends on the Ge-concentration. Samples with the highest Ge content demonstrate the transition temperature (Tc) of 1.2 K, attributed to increased Ga solubility, while samples with 70% of Si shows Tc around 100 mK. Notably, all samples achieved carrier concentrations over solid solubility, illustrating the effects of hyperdoping on superconductivity.

HL 6.3 Mon 15:30 H13

Direct printing of microlenses on hexagonal boron nitride to improve light outcoupling — •Daniel Klenkert[1,2], Paul Konrad[2], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]1Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg

Optically active defects in hexagonal boron nitride (hBN) have attracted wide research interest in the field of quantum technology. Solid immersion lenses can be employed in order to increase light outcoupling and thus the external quantum efficiency (EQE) of such defects. These lenses are, however usually created by etching them into the surface of the host material, which makes them rather unsuitable for 2D materials such as hBN.

Here we present an alternative approach: direct printing of polymer microlenses onto hBN using the two-photon polymerization technique. This strategy is not limited to bulk crystals, but can also be applied to thin films. Using a ceramic hybrid polymer with low fluorescence and high optical transparency, hemispherical lenses were directly printed on macroscopic hBN crystals and on thin flakes to demonstrate the feasibility and EQE enhancement of this approach.

HL 6.4 Mon 15:45 H13

Dynamical reorientation of spin multipoles in silicon carbide by transverse magnetic fields — •Alberto Hernández-Mínguez[1], Alexander V. Poshakinskiy[2], Michael Hollenbach[3], Paulo V. Santos[1], and Georgy V. Astakhov[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]ICFO-Institut de Ciències Fotòniques, Castelldefels, Spain — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The long-lived and optically addressable high-spin state of the negatively charged silicon vacancy (V_{Si}) in silicon carbide makes it a promising system for applications in quantum technologies. Most studies of its spin dynamics have been performed under external magnetic fields applied along the symmetry axis of the V_{Si} center. Here, we show that the application of a weak magnetic field perpendicular to the symmetry axis leads to a non-trivial behavior of the optically detected magnetic resonances (ODMRs) caused by the dynamical reorientation of the spin multipole under optical excitation. Particularly, we observe the inversion of the quadrupole-spin polarization in the excited state and the appearance of a dipole-spin polarization in the ground state. The latter is much higher than the thermal polarization and cannot be induced solely by optical excitation. Our theoretical model reproduces well all sharp features in the ODMR spectra and shine light on the complex dynamics of spin multipoles in these kinds of solid-state systems.

[1] A. Hernández-Mínguez *et al.*, Phys. Rev. Appl. **22**, 044021 (2024)

HL 6.5 Mon 16:00 H13

The hBN defects database for quantum applications — •Chanaprom Cholsuk[1,2], Asli Cakan[1,2], Sujin Suwanna[3], and Tobias Vogl[1,2,4] — [1]Department of Computer Engineering, School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [3]Optical and Quantum Physics Laboratory, Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand — [4]Abbe Center of Photonics, Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany

Hexagonal boron nitride (hBN) has emerged as a solid-state platform for hosting a variety of defects for quantum applications. Identifying

optimal defects for specific quantum applications has been challenging as some defects exhibit similar properties while others encounter strain. Comprehensive properties are therefore required. This work addresses this gap by utilizing density functional theory and open quantum system approaches to thoroughly characterize the properties of 257 defects and evaluate their potential for quantum emitter and quantum memory applications. This enables matching defects with suitable quantum applications. Furthermore, all findings are compiled into an accessible online database at https://h-bn.info, allowing one to compare our calculated optical fingerprints with experiments and other simulations. Consequently, this work enriches hBN defect resources, supporting progress in quantum technologies and defect identification.

HL 6.6 Mon 16:15 H13

Scanning NV center thermometry — Elias Sfeir[1], Maxime Rollo[1], Yoann Baron[2], Felipe Favaro de Oliveira[3], Gediminas Seniutinas[3], Marcelo Gonzàlez[3], Mathieu Mathieu[3], Patrick Maletinsky[3,4], Jean-Baptiste Jager[5], Jean-Michel Gérard[5], Vincent Jacques[1], •Aurore Finco[1], and Isabelle Robert-Philip[1] — [1]Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France — [2]Univ. Grenoble Alpes, CEA, LETI, Grenoble, France — [3]Qnami, Muttenz, Switzerland — [4]Department of Physics, University of Basel, Basel, Switzerland — [5]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, Grenoble, France

Scanning NV center microscopy relies on a single nitrogen-vacancy (NV) defect in diamond as a quantum sensor for scanning probe experiments. It is now routinely used as a powerful magnetometry technique, and its functionalities can be extended to temperature measurements by exploiting the temperature dependence of the NV electron spin resonance (ESR) frequency. In this work, we show how to simultaneously map the Joule heating and the Oersted field generated by an electrical current flowing through a semiconductor nanowire with a scanning NV center microscope. Our results highlight that the component of the magnetic field perpendicular to the NV center quantization axis competes with the effect of temperature on the NV ESR frequency, making quantitative temperature measurements challenging. Therefore, we finally propose solutions to improve the overall performances of the technique through the design of optimized diamond probes.

15 min. break

HL 6.7 Mon 16:45 H13

Luminescence of electron and ion beam irradiated hBN — •Jan Böhmer, Annkathrin Köhler, Christian T. Plass, and Carsten Ronning — Friedrich Schiller University, Jena, Germany

Defect centers in solid state materials have emerged as promising candidates for quantum emitters. Here, hexagonal boron nitride (hBN) has attracted much interest as an interesting material for the realization of room temperature single photon emitters (SPEs). Emitting defects can be specifically created by irradiation of hBN flakes and nanoparticles with (focused) electron and ion beams, which allows to modify the luminescence properties of the hBN samples and fabricate targeted localized SPEs. The effects of the irradiation on the luminescence spectrum were investigated using micro photoluminescence (μPL). The nature and applicability for SPEs were determined by $g_{(2)}$-autocorrelation measurements as a function of the irradiation parameters.

HL 6.8 Mon 17:00 H13

Strain-induced tuning of quantum emitters in hexagonal boron nitride — •Tjorben Matthes[1,2], Anand Kumar[1,2], Mohammad Nasimuzzaman Mishuk[1,2], and Tobias Vogl[1,2] — [1]Department of Computer Engineering, TUM School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

In this talk, we will show our recent progress in controlling the emission characteristics of our single photon emitters in hexagonal boron Nitride (hBN).

We have previously demonstrated our results on the polarisation characteristics of both the absorption and the emission characteristics of our single photon emitters. By conducting a statistical analysis of a large array of emitters, we found some unexpected results that indicate a shift of the emission axes in one direction compared to the crystal axes. We suspected a strain induced by the exfoliation process as the cause. We, therefore, conduct now further tests deliberately inducing strain into the hBN flakes in which the emitters are embedded.

HL 6.9 Mon 17:15 H13

Impact of a magnetic field on low-temperature photoluminescence of indium-doped silicon — •Kevin Lauer[1,2], Mario Bähr[1], Richard Grabs[1], Frank Long[1,3], Martin Kaleta[1], Andreas Frank[1], Thomas Ortlepp[1], Katharina Peh[2], Noah Stiehm[2], Rüdiger Schmidt-Grund[2], Dirk Schulze[2], and Stefan Krischok[2] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [3]Universität Göttingen, Göttingen, Germany

Acceptor-interstitial silicon (ASi-Sii)-defects [1] were proposed to be responsible for a gain loss in low-gain avalanche detectors (LGAD) and for an efficiency loss in silicon solar cells. Recently, it was speculated that this defect category could be relevant for silicon-based quantum technology, as well. To advance the understanding of these defects in silicon with respect to their potential use as qubits, low-temperature photoluminescence (PL) measurements are performed while subjecting the sample to magnetic fields. Silicon samples with and without indium doping were treated by a temperature quenching step to generate ASi-Sii-defects. The ASi-Sii-defect generation was done using a local laser quenching method as well as using a Bunsen burner with subsequent water quenching. As expected, the integrated PL intensity increased after this generation process. While the sample is subjected to magnetic fields, the integrated PL intensity changes significantly. Differences between samples with and without indium doping will be discussed. [1]K. Lauer et al., Phys. Status Solidi A, 219 (2022) 2200099

HL 6.10 Mon 17:30 H13

Fabrication, characterization and deformation of Si/SiGe membranes for spin qubit devices — •Lucas Marcogliese[1], Ouviyan Sabapathy[1], Rudolf Richter[2], Dominique Bougeard[2], and Lars R. Schreiber[1,3] — [1]JARA-FIT Institute for Quantum Information, Aachen, Germany — [2]University of Regensburg, Regensburg, Germany — [3]ARQUE Systems GmbH, Aachen, Germany

The energy separation between the two lowest lying energy states in silicon, known as valley splitting, has been shown to have a significant impact on dephasing times, readout and shuttling fidelities of spin qubits in Si/SiGe. Greater control over the strain tensor field may be decisive for deterministic valley splitting enhancement in the presence of alloy disorder. Here, we demonstrate the fabrication of SiGe/Si/SiGe quantum well membranes suspended by the handle wafer via wet etching. Relying on SiGe as an etch stop, the robust and reproducible process yields membranes down to micrometer thicknesses. Raman maps confirm that etching preserves epitaxial tensile strain in the quantum well. Remarkably, they reveal that the in-plane strain components generated by the cross-hatch pattern typical of Si/SiGe heterostructures on bulk substrates disappear on etched membranes. To probe their elastic properties, the membranes are stressed by loading with a profilometer stylus at room temperature. We envision the Si/SiGe membrane as a flexible scientific platform for investigating novel, advanced valley splitting enhancements techniques, required for scalable Si/SiGe quantum computing with electron spins.

HL 6.11 Mon 17:45 H13

Design and optimization of bimodal cavities coupled to multi-level quantum systems — •Oscar Camacho Ibarra, Jan Gabriel Hartel, Atzin Ruiz Perez, Sonja Barkhofen, and Klaus Jöns — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany

Photonic integrated cavities are essential building blocks for qubit-controlled switches, routers, and gates in quantum networks and quantum information processing. These devices rely on the integration of multi-level quantum systems coupled to multiple photonic modes inside a cavity. Thus, the present work introduces a systematic workflow for the design of bimodal cavities by employing one-dimensional crossed photonic crystal nanobeam cavities with non-zero cavity lengths. By optimizing three key parameters*the periodicity, a single feature size of the hole shape, and the central cavity length*we establish a robust methodology for designing crossed nanobeam cavities. This approach supports configurations with either matching or mismatched resonance frequencies, offering flexibility for diverse quantum applications. References [1]* Mikkel Heuck, Kurt Jacobs and Dirk R. Englund. Controlled-Phase Gate Using Dynamically Coupled Cavities and Optical Nonlinearities. Phys. Rev. A 109, 062620 (2024). [2]* Luiz O. R. Solak, Daniel Z. Rossatto, and Celso J. Villas-Boas,

Universal quantum computation using atoms in cross-cavity systems. Phys. Rev. A 109, 062620 (2024).

HL 6.12 Mon 18:00 H13

In Situ Defect Density Determination of Spin Defects in Hexagonal Boron Nitride — Atanu Patra[1], •Paul Konrad[2], Andreas Sperlich[2], Timur Biktagirov[3], Thinh Tran[4], Igor Aharonovich[4], Sven Höfling[1], and Vladimir Dyakonov[2] — [1]Technische Physik, Julius-Maximilians-University Würzburg, 97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-University Würzburg, 97074 Würzburg — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [4]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

In recent years, the negatively charged boron vacancy (V_B^-) spin defects in hexagonal boron nitride (hBN) caught attention for their sensitivity to environmental parameters such as magnetic field, temperature, and pressure, making them ideal for quantum sensing. The optical emission from these defects, crucial for applications, depends on their density, which could -so far- not be determined directly for thin flakes. Our study identifies distinct Raman modes alongside the E_{2g} peak in defect-enriched hBN. Polarization-dependent Raman measurements reveal that these modes arise from atomic vibrations associated with the V_B^- defects. Additionally, we corroborate this result by density functional theory. We investigate the interdependent relationship between the vibronic states and defect density and obtain a universally applicable method to directly determine the absolute spin-defect density in flakes by Raman spectroscopy alone.

HL 6.13 Mon 18:15 H13

Electric-circuit realization of the Floquet-SSH-Model — •Christine Barko[2], Alexander Stegmaier[1], Alexander Fritzsche[1], Riccardo Sorbello[1], Martin Greiter[1], Hauke Brand[2], Maximilian Hofer[2], Udo Schwingenschlögl[3], Roderich Moessner[4,5], Ching Hua Lee[6], Alexander Szameit[5,7], Andrea Alù[8,9], Tobias Kiessling[2,5], and Ronny Thomale[1,5] — [1]Physikalisches Inst. (TP1), Universität Würzburg, Würzburg, Germany — [2]Physikalisches Inst. (EP3), Universität Würzburg, Würzburg, Germany — [3]Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, Dresden, Germany — [5]Würzburg-Dresden Cluster of Excellence ct.qmat, Würzburg, Germany — [6]Department of Physics, National University of Singapore, Singapore — [7]Institute of Physics, University of Rostock, Rostock, Germany — [8]Photonics Initiative, Advanced Science Research Center, City University of New York, New York, USA — [9]Physics Program, Graduate Center, City University of New York, New York, USA

We build Floquet-driven capactive circuit networks to realize topological states of matter in the frequency domain. We find the Floquet circuit network equations of motion to reveal a potential barrier which effectively acts as a boundary in frequency space. By implementing a Su-Shrieffer-Heeger Floquet lattice model and measuring the associated circuit Laplacian and characteristic resonances, we demonstrate how topological edge modes can nucleate at such a frequency boundary.

HL 6.14 Mon 18:30 H13

Erbium dopants in nanophotonic resonators — •Andreas Gritsch, Alexander Ulanowski, Stephan Rinner, Johannes Früh, Jakob Pforr, and Andreas Reiserer — Technical University of Munich, TUM School of Natural Sciences and Munich Center for Quantum Science and Technology (MCQST), 85748 Garching, Germany

Optically addressable spin qubits are pristine candidates for large-scale quantum networks [1] and modular quantum computing architectures [2]. Erbium dopants are the only emitter with a coherent optical transition in the minimal-loss-band of optical fibers. In silicon, erbium integration is compatible with industrial-grade nanofabrication processes [4]. In nanophotonic resonators efficient spin-photon interfaces can be realized, in which about ten single dopants can be resolved with Purcell enhancement up to 177. Their spin state can be initialized and read out with a combined fidelity of 87%. This spin further exhibits a second-long lifetime and a Hahn-echo coherence time of 48 s [4]. We further investigate the optical coherence and the spectral multiplexing capabilities in our silicon devices, which allows a detailed comparison to our experiments with YSO membranes integrated into Fabry-Perot resonators [5].

[1] A. Reiserer, Rev. Mod. Phys. 94, 041003 (2022). [2] S. Simmons, PRX Quantum 5, 010102 (2024). [3] S. Rinner, et al., Nanophotonics 12 (2023). [4] A. Gritsch, et al., arXiv:2405.05351 (2024), Nat. Commun., (in press). [5] A. Ulanowski, et al., Advanced Optical Materials 12 (2024).

HL 7: Semiconductor Lasers

Time: Monday 15:00–15:45 Location: H14

HL 7.1 Mon 15:00 H14

Development and Analysis of a VECSEL based on InGaAs Quantum Dots for Emissions in the Telecom O-Band — •Justus Unfried, Philipp Noack, Rebecca Rühle, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The advancement of sophisticated laser technologies for high-resolution spectroscopy and sensing applications has stimulated interest in versatile, high-performance light sources. Vertical External-Cavity Surface-Emitting Lasers (VECSELs) based on InGaAs quantum dots (QDs) are promising for emissions in the telecommunications O-band and offer broad wavelength tunability, high output power, and excellent beam quality. This study focuses on optimizing QD layers through metal-organic vapor-phase epitaxy (MOVPE), utilizing the Stranski-Krastanov growth mode, followed by laser performance characterization. To enhance QD density and emission characteristics, the gallium precursor was substituted with TEGa, exhibiting a higher decomposition rate at lower growth temperatures. The indium supply was modified, and the duration of the arsine interruption following QD deposition was examined to increase density and reduce large In-clusters. Subsequently, 12 of these high-density QD layers are deposited on a distributed Bragg reflector (DBR) structure, completing the VECSEL. This laser development is accompanied by structural and performance characterizations.

HL 7.2 Mon 15:15 H14

Comparison between a 675nm and 532nm pumped 4x3 InGaAsP QW VECSEL emitting at around 760nm in a V-Shaped resonator — •Rebecca Rühle[1], Maxim Leyzner[2], Marwan Abdou Ahmed[2], Thomas Graf[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Strahlwerkzeuge, Universität Stuttgart, Pfaffenwaldring 43, 70569 Stuttgart, Germany

The quantum defect between the emission and the pump wavelengths has a substantial impact on the performance of a vertical external-cavity surface-emitting lasers (VECSEL). An increase in the wavelength of the pump laser should result in an improvement in thermal behavior and the laser performance. One disadvantage is that the pump absorption is reduced, given that the pump energy is typically below the barrier bandgap. In our previous studies, the GaInP barrier of our InGaAsP VECSEL structure was modified to absorb pump light at a wavelength of 675nm. Power measurements were conducted with a 675nm pump laser and a 532nm pump laser, employing the aforementioned adapted structure. By varying the reflectivity of the outcoupling mirror in the V-shaped resonator, we gain further insight into the absorption characteristics within the active region of the VECSEL. Due to the specifications of the laser source, the pump spot size was approximately 310μmx230μm, resulting in a multimode emission from the VECSEL rather than single mode for both pumplasers.

HL 7.3 Mon 15:30 H14

Quantum optical validation of high-β lasing in monolayer-

based self-assembled photonic-defect nanocavities — •Aris Koulas-Simos[1], Chirag Palekar[1], Kartik Gaur[1], Imad Limame[1], Bárbara Rosa[1], Cun-Zheng Ning[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Teschnische Universität Berlin, 10623 Berlin, Germany — [2]College of Integrated Circuits and Optoelectronic Chips, Shenzhen Technology Univesity, Shenzhen 518118, China

Nanolasers based on transition metal dichalcogenides have garnered substantial research interest for innovative photonic applications. This study presents the fabrication of multiple self-assembled photonic defect nanocavities within a single, fully encapsulated WSe_2 monolayer integrated into a dielectric distributed Bragg reflector (DBR) structure. Spontaneously formed bubbles during the encapsulation process lead to the generation of photonic-defect nanocavities in the DBR. These structures achieve strong optical lateral confinement and exhibit size-dependent optical characteristics, as confirmed by μPL-measurements in both the real and k-space and numerical cavity simulations. Optical power-dependent investigations conducted at cryogenic temperatures reveal lasing behavior, evidenced by a distinct kink in the input-output curve, accompanied by slight linewidth narrowing and a lineshape transition in two specific devices. Finally, photon-autocorrelation measurements performed on one of these devices provide unequivocal confirmation of a lasing transition [1].

[1] A. Koulas-Simos et al., Laser & Photonics Rev., 2400271 (2024).

HL 8: 2D Semiconductors and van der Waals Heterostructures II

The session covers the physics of emerging 2D materials.

Time: Monday 15:00–16:15 Location: H15

HL 8.1 Mon 15:00 H15

atomic and electronic structures of colloidal ultrathin PbSe nanoplatelets — •huu thoai ngo[1,2], leon biesterfeld[3], ahmed addad[1], bruno grandidier[1], christophe deere[1], jannika lauth[3], and louis biadala[1] — [1]Université de Lille, CNRS, Centrale Lille, Université Polytechnique Hauts-de-France, Junia-ISEN, UMR 8520-IEMN, INRAE, UMR-8207, UMET- Unité Matériaux et Transformations, F-59000 Lille, France. — [2]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany. — [3]Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Callinstr. 3A, D-30167 Hannover, Germany

Two-dimensional (2D) PbSe nanoplatelets (NPLs) are promising materials for lighting technologies due to their efficient and tunable photoluminescence (PL), such as narrow PL emission reaching telecom bands. However, the electronic properties of single NPLs remain underexplored, limiting insights into quantum confinement effects. Here, we investigate the structural and electronic properties of ultrathin PbSe NPLs using low-temperature scanning tunneling microscopy (LT-STM). STM images confirm flat 2D morphologies at various thicknesses while tunneling spectra reveal pronounced quantum confinement along the thickness, resulting in bandgap shifts. High-angle annular dark-field scanning transmission electron microscopy confirms the rock-salt crystal structure, providing atomic-level insights. Additionally, tight-binding calculations demonstrate lateral quantum confinement effects, showing that in-plane dimensions influence electronic properties.

HL 8.2 Mon 15:15 H15

Modifying properties of 2D transition metal dichalcogenides by confined-space annealing — •Christian Tessarek, Christian Petersen, Tim Grieb, Florian F. Krause, Alexander Karg, Christian Habben, Andreas Rosenauer, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

2D transition metal dichalcogenides (TMDs) can be grown by different methods, e.g. chemical vapor or atomic layer deposition (ALD) [1]. Subsequent annealing is often applied to improve the properties of the as-grown 2D layers. Decomposition of TMD layers due to desorption of chalcogenides usually limits the temperature range. Higher annealing temperatures are possible in a chalcogene containing atmosphere but require special safety requirements of the annealing equipment.

In this study, a confined-space annealing (CSA) approach is demonstrated and realized by a close contact face-to-face sample arrangement of TMD layers on SiO_2/Si or graphene substrates. CSA is performed in vacuum or in an inert gas atmosphere without using additional chalcogene containing precursors. Such sample arrangement strongly reduces chalcogene outdiffusion from the confined space and allows annealing at higher temperatures and longer durations. The influence of CSA parameters is investigated with respect to structural and optical properties of the TMDs and compared to a standard annealing process of uncovered layers. It will also be shown that CSA can be used for conversion of MoS_2 to ternary $Mo(S,Se)_2$ and binary $MoSe_2$.

[1] C. Tessarek et al., 2D Mater. **11**, 025031 (2024).

HL 8.3 Mon 15:30 H15

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

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

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

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

HL 8.4 Mon 15:45 H15

Biaxial Compressive Strain Tuning of Quantum Properties in 2D Materials — •Eudomar Rafael Henriquez Guerra[1,3], Lisa Almonte[1,3], Hao Li[4], Daniel Elvira[3], Reyes Calvo[1,2,3], and Andres Castellanos Gomez[4] — [1]BCMaterials, Basque Center for Materials, Applications and Nanostructures — [2]Ikerbasque, Basque Foundation for Science — [3]Depto. de Física Aplicada, Instituto Universitario de Materiales, Universidad de Alicante — [4]2D Foundry Group, Instituto de Ciencia de Materiales de Madrid, CSIC

This study investigates the impact of biaxial compressive strain on 2D materials at cryogenic temperatures, focusing on single-layer transition metal dichalcogenides (TMDs) and multilayered NbSe2. While tensile strain has been widely explored, compressive strain at low temperatures remains underexplored, despite its potential to significantly alter quantum properties such as magnetic and superconducting phase transitions. We show that biaxial compressive strain, induced by the thermal expansion mismatch between the polymer substrates and TMDs, leads to dramatic shifts in exciton energy and gauge factors, surpassing previous compressive strain effects. Moreover, we observe a consistent reduction in the superconducting critical temperature of NbSe2 flakes, with the most pronounced changes in thinner samples. Remarkably, this effect is still noticeable even for NbSe2 flakes as thick as 86 nm. These results highlight a powerful and cost-effective method for tuning phase transitions and other quantum phenomena in 2D materials at low temperatures.

HL 8.5 Mon 16:00 H15

Two-dimensional semiconductor with tunable bandgap close to the full visible spectrum: a MOCVD study — •Nils Langlotz, Robin Günkel, Tigmanshu Sundiyal, Oliver Massmeyer, Jürgen Belz, and Kerstin Volz — Department of Physics and Material Sciences Center, Philipps-University Marburg, Germany

Two-dimensional (2D) semiconductors have attracted considerable attention due to their extraordinary thickness-dependent properties. III-VI compounds such as GaSe or GaS exhibit a unique Mexican hat band structure with a van Hove singularity near the valence band maxima (VBM) at the Γ point. Furthermore, 2D GaSe and GaS as bulk material have a direct band gap of 2.0 eV and 2.5 eV, respectively, making a dilute $GaSe_xS_{1-x}$ system a tunable LED in the visible regime. Tuning the band gap in the few layer regime is also possible, but the indirect band gap has to be overcome, which is suggested by doping. Metal organic chemical vapour deposition (MOCVD) is used for the growth of bulk GaSe, GaS and $GaSe_xS_{1-x}$ on sapphire (0001). Growth for all materials was performed in an AIX200GFR at 50 mbar at 500°C in a flow modulated growth mode where the first pulse is 30 s of the gallium species and the second pulse is 30 s of selenium or sulphur, repeated for 150 cycles for the pure crystals. For the diluted crystal the second pulse is replaced by $(30-x)$ s of selenium followed by x seconds of sulphur. The organometallic precursors used were tri-tertiarybutyl-gallium (TTBGa), di-iso-propyl-selenide (DiPSe) and tertiarybutyl-sulphide (TBS). Raman spectroscopy is used to verify the selenium/sulphur incorporation.

HL 9: Oxide Semiconductors I

Time: Monday 15:00–16:30 Location: H17

HL 9.1 Mon 15:00 H17

Nitrogen Doping of Sputtered $BiVO_4$ Thin Films — •Hannah Sassenfeld[1,2], Tsedenia Zewdie[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, D-85748 Garching, Germany

Bismuth vanadate ($BiVO_4$) is a promising photoanode material for photoelectrochemical (PEC) water splitting, given its suitable band gap (≈2.5 eV) and valence band maximum position relative to the water oxidation potential. Reducing the band gap of $BiVO_4$ can lead to a more effective utilization of the solar spectrum. One strategy towards band gap reduction is nitrogen incorporation, as previously reported by Irani et al. [1] and Kim et al. [2]. While both studies observe reduced band gaps, they do not agree on how nitrogen is incorporated into $BiVO_4$ and whether it improves or deteriorates PEC performance. To shed light onto the nature and effects of nitrogen incorporation, we use well-controlled reactive co-sputter deposition of $BiVO_4$ in nitrogen-containing environments (N:$BiVO_4$). Adjusting the amount of nitrogen in the reactive gas mixture and post-annealing treatments allow us to control the amount of incorporated nitrogen. Using this systematic sample library of N:$BiVO_4$, we interrogate the optical and structural properties of N:$BiVO_4$, its composition and electronic structure, and evaluate the impact of nitrogen incorporation on PEC performance.

[1] Irani et al. Solar RRL 4.1 (2020): 1900290. [2] Kim et al. Nature communications 6.1 (2015): 8769.

HL 9.2 Mon 15:15 H17

Plasma Plume Deflection and Target Surface Roughness During Pulsed Laser Deposition of Functional Oxides — •Jonas Elz, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Pulsed laser deposition (PLD) is a highly flexible, fast and reproducible physical vapor deposition technique that uses a pulsed laser to evaporate a target material, producing an excited laser-induced plasma. Although simple in set-up, modeling the ablation process is difficult because of its non-equilibrium nature due to the high pulse energy incident on a short time scale (20 ns laser pulse width). Ablation of any target material requires optimization of the process parameters. Some targets used in PLD develop a rough surface structure upon longer use that causes the plasma plume to deflect toward the incoming laser beam during the ablation process. Typically, the plume deflection increases until a stable surface morphology is reached. In this work, we present a comparison of the plasma plume deflection with surface roughness and morphology of different PLD targets as measured by laser scanning microscopy. A Python script is used to evaluate plume images to determine the deflection angle.

HL 9.3 Mon 15:30 H17

Analysis of film thickness distributions for combinatorial pulsed laser deposition — •Clemens Petersen, Marius Grundmann, and Holger von Wenckstern — Universität Leipzig Felix-Bloch-Institut für Festkörperphysik, Leipzig, Deutschland

Recently combinatorial deposition methods have increasingly gained scientists* attention, due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. They enable fast screening of material properties of multinary material systems using just a single sample. By employing pulsed laser deposition with our segmented target approach [1] we realized the deposition of α-$(Al_xGa_{1-x})_2O_3$ with continuous composition spread over the whole composition range on a single 2-inch sapphire wafer [2]. Accompanied by the usage of high-throughput measurements such as spectroscopic ellipsometry and X-ray diffraction, the characterization of physical properties with high chemical resolution and comparably low efforts becomes feasible.

Here we utilize a predictive numerical model, based on the corrected plasma expansion description of Anisimov *et al.* [3], for the calculation of binary growth rates of group-IIII and transition metal sesquioxides. Further the model can be applied to predict and model elemental composition and thickness distributions of ternary alloys for these materials. [1] H. von Wenckstern *et al.*, pss(b), Vol. 257, 1900626 [2] A. Hassa *et al.*, pss(b), Vol. 258, 2000394 [3] S. I. Anisimov *et al.*, Phys. rev. B, Vol 48, 12076.

HL 9.4 Mon 15:45 H17

Influence of different gate metals on α-Ga_2O_3 MESFET device performance — •Sebastian Köpp, Clemens Petersen, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

We present metal-semiconductor field effect transistors (MESFET) on α-Ga_2O_3 grown by pulsed laser deposition in a two-step process on Al_2O_3 [5]. The MESFETs exhibit high on/off ratios above 9 orders of magnitude and subthreshold swings as low as 100 mV/dec. We evaluate different gate materials in an effort to optimize device switching and breakdown behaviour.

With its ultra-wide bandgap of 5.3 eV to 5.6 eV [1,2] and a high predicted breakdown field of 10 MV/cm [3], α-Ga_2O_3 is a promising material for high-power devices, as well as deep-UV photodetectors. α-Ga_2O_3, being isostructural to aluminium oxide, allows for heteroepitaxial growth on cost-efficient sapphire substrates, and also opens up the option of α-$(Al_xGa_{1-x})_2O_3$ alloys [4], potentially pushing device performance even further.

[1] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[2] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)
[3] M. Biswas and H. Nishinaka, APL Mater. 10, 060701 (2022)
[4] J. Steele *et al.*, APL Mater. 12, 041113 (2024)
[5] S. Vogt *et al.*, Phys. Status Solidi A, 220 2200721 (2023)

HL 9.5 Mon 16:00 H17

Adsorption-controlled growth of κ-Ga2O3 — •Alexander Karg[1], Niklas Krantz[1], Manuel Alonso-Orts[1,2], Marco Schowalter[1,2], Patrick Vogt[1,3], Andreas Rosenauer[1,2], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany — [3]Max Planck Institute for solid state research, Heisenbergstraße 1, 70569 Stuttgart, Germany

The ultra-wide band gap semiconductor Ga2O3 can crystallize in at least 5 different polymorphs. For one of these, the metastable κ-Ga2O3, a spontaneous polarization along the c-axis is predicted [1]. Utilizing this property in heterostructure devices requires the formation of sharp, distinct interfaces between different alloyed layers to achieve high sheet carrier densities.

The recent development of suboxide MBE (S-MBE) has enabled the adsorption-controlled growth of Ga2O3 thin films [2]. In this contribution, S-MBE is specifically applied to the growth of metastable,

orthorhombic κ-Ga2O3. The growth process, phase stabilization, and their impact on layer properties are analyzed in detail. This is combined with the use of indium as surfactant. Additionally, the study is complemented by the realization of κ-Ga2O3-based heterostructures using suboxide MBE [3].

[1] Maccioni et al., Appl. Phys. Express 9, 041102 (2016);[2] Vogt et al., U.S. Patent No. 11,462,402 (2022);[3] Karg et al., APL Mater. 11, 091114 (2023)

HL 9.6 Mon 16:15 H17

Realization of highly rectifying pn-heterojunctions on pulsed laser deposited α-Ga_2O_3 thin films — •Paul Bokemeyer, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — University Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnestr. 5, Leipzig, Germany

The wide band gap of about 5.3 eV[1], the possibility for adjusting the band gap energy by alloying with isostructural aluminum oxide or indium oxide[1] and a high expected breakdown field of up to 10 MV/cm[2], renders the corundum α-phase of Ga_2O_3 interesting for high power applications. We present lateral p^+n-heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition(PLD) using a two step approach[3]. Room temperature deposited ZnCoO(ZCO) (PLD), NiO (PLD) and CuI (PLD and sputtering) were used as p^+-type materials. We further investigated the influence of a remote oxygen plasma treatment prior to the deposition of the p-type layers on the device performance. High current rectification ratios of of 8.2 (ZCO), 7.8 (NiO), and 5.1 (CuI) orders of magnitude at ± 3V were achieved. Additionally, α-Ga_2O_3:Zr junction-field-effect-transistors(JFETs) with ZCO and NiO as gate materials were fabricated, yielding on/off ratios of more than 9 orders of magnitude and sub-threshold-swings down to 119 mV/dec.

[1] A. Hassa et.al., J.Phys. D: Appl. Phys. **54**, 223001 (2021)
[2] M. Biswas et al., APL Mater. **10**, 060701 (2022)
[3] S. Vogt et al., Phys. Status Solidi A, **220** 2200721 (2023)

HL 10: Spin-Dependent Phenomena in 2D (joint session MA/HL)

Time: Monday 15:00–17:15 Location: H19

HL 10.1 Mon 15:00 H19

Magnetoelectric behavior of breathing kagomé monolayers of Nb3(Cl,Br,I)8 from first-principles calculations — •John Mangeri — Technical University of Denmark, Kongens Lyngby, Denmark

We apply density functional theory to explore the magnetoelectric (ME) properties of two-dimensional Nb3(Cl,Br,I)8. These compounds have recently been proposed to exhibit coupled ferroelectric and ferromagnetic order leading to a switchable anomalous valley Hall effect (AVHE). Using both spin-spiral and self-consistent spin-orbit coupled calculations, we predict an in-plane 120 degree cycloid of trimerized spins as the ground state for Nb3Cl8. For Nb3Br8 and Nb3I8 we find long period incommensurate helical order. We calculate a number of magnetic properties such as the exchange constants, orbital magnetization, and Weiss temperatures. It is then shown that, despite having both broken inversion and time-reversal symmetry, the proposed AVHE and linear ME response are forbidden by the presence of helical order in the ground state. In addition, the computed switching trajectory demonstrates that it is unlikely that the polar state of the monolayers can be switched with a homogeneous electric field due to an unusual equation of state of the out-of-plane dipole moment. Nevertheless, we highlight that in the presence of a strong electric field, the trimerized spins in Nb3Cl8 will exhibit a magnetic phase transition from the 120 degree cycloid to out-of-plane ferromagnetic order, which restores the symmetry required for both AVHE and linear ME effects.

HL 10.2 Mon 15:15 H19

Ab-initio Investigation of two-dimensional Fe-Sn Kagome lattice with Nb doping — •Gérald Kämmerer[1,2] and Sinéad Griffin[2] — [1]Faculty of Physics, University of Duisburg-Essen — [2]Lawrence Berkeley National Laboratory (LBNL), Berkeley

This research investigates Fe-Sn-based kagome compounds for green energy applications, focusing on their magnetic and electronic properties, particularly in spintronics and phononics. We are investigating tunable properties in Fe_3Sn. We aim to control spin states in 2D magnetic systems by studying doped variants (Nb) in Kagome lattices to uncover topological electronic states, including Dirac fermions and flat bands.

Using first-principles calculations, we analyse impurity interactions in 2D lattices using VASP. By comparing experimental data with our computational results, this study aims to provide insights into dopant-controlled quantum states and improve material performance in electronic applications.

The financial support of the DFG within the SFB 1242 and the computational time on the LBNL supercomputer system are gratefully acknowledged.

HL 10.3 Mon 15:30 H19

Spin polarization of the two-dimensional electron gas at the EuO/$SrTiO_3$ interface — •Paul Rosenberger[1,2], Andri Darmawan[3], Olena Fedchenko[1], Olena Tkach[1], Serhii V. Chernov[4], Dmitro Kutnyakhov[4], Moritz Hoesch[4], Markus Scholz[4], Kai Rossnagel[4,5], Rossitza Pentcheva[3], Gerd Schönhense[1], Hans-Joachim Elmers[1], and Martina Müller[2] — [1]JGU Mainz, Germany — [2]Uni Konstanz, Germany — [3]UDE, Duisburg, Germany — [4]DESY, Hamburg, Germany — [5]CAU Kiel, Germany

Spin-polarized two-dimensional electron gases (2DEGs) are of particular interest for functional oxide electronics applications. Here, we use magnetic circular dichroism in the angular distribution (MCDAD) of photoemitted electrons to investigate whether and how the induced spin polarization of the redox-created 2DEG at the EuO/$SrTiO_3$ (001) interface depends on the dimensionality of the strongly ferromagnetic ($7\,\mu_B/f.u.$) EuO layer [1]. Samples with EuO thicknesses ranging from one to four monolayers were studied. We show that the EuO/STO interfacial 2DEG becomes spin-polarized starting from a threshold EuO thickness of only two monolayers. Experimental data are complemented by DFT+U calculations. Our results, and the potential to enhance the magnetic order of EuO by other proximity effects [2], indicate that the EuO/STO interface is an ideal template for creating functional spin-polarized 2DEGs for application in oxide electronics.

[1] Rosenberger *et al.*, arXiv:2410.23804 (2024).
[2] Rosenberger *et al.*, Sci. Rep. **14**, 21586 (2024).

HL 10.4 Mon 15:45 H19

***Ab initio* calculation of Spin-Orbit torques in 2D magnets** — •Gusthavo Brizolla and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The interplay of spin-orbit coupling and magnetism in two-dimensional materials and their heterostructures presents exciting opportunities for advancing next-generation spintronic devices. In this work, we investigate the role of proximity effects in generating spin-orbit torques (SOTs) in Fe_3GeTe_2 (FGT) and FGT-based van der Waals heterostructures. Using a tight-binding Hamiltonian derived from first-principles calculations via the Wannierization procedure, we evaluate the torkances within the linear response regime using the Kubo formalism. Our results reveal key mechanisms underlying the generation of torques driven by spin accumulation, elucidating the fundamental physics of SOTs in these systems.

This research has been supported by 2D SPIN-TECH.

HL 10.5 Mon 16:00 H19

Unveiling Long-range Magnetic Textures in Twisted Moiré Antiferromagnets — •King Cho Wong[1], Ruoming Peng[1], Xiaodong Xu[3], Elton Santo[2], Adam Wei Tsen[4], Rainer Stoehr[1], and Joerg Wrachtrup[1] — [1]3rd Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]University of Edinburgh, United Kingdom — [3]University of Washington, USA — [4]University of Waterloo, Canada

Stacking two-dimensional (2D) materials offers a controllable and versatile platform to engineer interlayer interactions, unveiling numerous intriguing correlated and topological states. Recent progresses in twisted 2D magnets have revealed periodic ferromagnetic domains due

to the local Moiré stacking. In this study, we employed scanning quantum microscopy to investigate local magnetic responses of twisted double bilayer chromium triiodide (tDB CrI3). We observed unexpected antiferromagnetic textures with periods more than 300 nm at the 1.1° twisted devices, which are significantly exceeding the corresponded Moiré size of about 30 nm. These periodic magnetic textures are setting atop randomly distributed ferromagnetic domains with net two-layer magnetization of 30 uB/nm^2 and antiferromagnetic domains with magnetization of 0 uB/nm^2. Our findings suggest that strong magnetic competition at small twisted angles (<2°) can extend magnetic textures beyond the Moiré size, leading to the emergence of Néel skyrmions after field cooling.

HL 10.6 Mon 16:15 H19

Spin model of graphene triangulenes embedded in hexagonal boron nitride — •Dániel Tibor Pozsár[1,3,4,5], László Oroszlány[1,2,3], and Viktor Ivády[1,4,5,6] — [1]Department of Physics of Complex Systems, Eötvös Loránd University, Egyetem tér 1-3, H-1053 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]TRILMAX Consortium, Twinning, Horizon Europe, Budapest, Hungary — [4]QUEST projec, Twinning, Horizon Europe, Budapest, Hungary — [5]MTA*ELTE Lendület "Momentum" NewQubit Research Group, Pázmány Péter, Sétány 1/A, 1117 Budapest, Hungary — [6]Department of Physics, Chemistry and Biology, Linköping University, SE-581 83 Linköping, Sweden

We are investigating triangulene shaped substitutional defects in hexagonal boron nitride filled with carbon atoms. We show how the triangulene shaped defects encompass magnetic moments and with ab initio methods we build Heisenberg like classical spin models representing their interactions. We show how different lattice terminations and sizes impact the magnetic properties of the system.

HL 10.7 Mon 16:30 H19

Realizing Spin-3/2 AKLT State for Quantum Computation with Tetrapod Architectures — •Claire Benjamin[1], László Oroszlány[1,2], Dániel Varjas[3], and Gábor Széchenyi[1] — [1]Department of Physics of Complex Systems, Eötvös University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary

Using a novel tetrapod (5-site cluster) architecture, we implement spin-3/2 degrees of freedom in a semiconductor quantum bit platform. This framework enables us to construct a tunable artificial spin system that can realize the two-dimensional Affleck-Kennedy-Lieb-Tasaki (AKLT) state on a honeycomb lattice, known to be a universal resource for measurement-based quantum computation. We assess the model's robustness and feasibility for measurement based quantum computing using semi-analytic perturbation theory and numerical calculations.

HL 10.8 Mon 16:45 H19

Anomalous quantum oscillations from boson-mediated interband scattering — •Léo Mangeolle[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Quantum oscillations (QO) in metals refer to the periodic variation of thermodynamic and transport properties as a function of inverse applied magnetic field. QO frequencies are normally associated with semi-classical trajectories of Fermi surface orbits but recent experiments challenge the canonical description. We develop a theory of composite frequency quantum oscillations (CFQO) in two-dimensional Fermi liquids with several Fermi surfaces and interband scattering mediated by a dynamical boson, e.g. phonons or spin fluctuations. Specifically, we show that CFQO arise from oscillations in the fermionic self-energy with anomalous frequency splitting and distinct strongly non-Lifshitz-Kosevich temperature dependencies. Our theory goes beyond the framework of semi-classical Fermi surface trajectories highlighting the role of many-body effects. We provide experimental predictions and discuss the effect of non-equilibrium boson occupation in driven systems.

HL 10.9 Mon 17:00 H19

Identifying the Origin of Thermal Modulation of Exchange Bias in $Fe_3GeTe_2/MnPS_3$ van der Waals Heterostructures — Aravind Puthirath Balan[1], •Aditya Kumar[1], Patrick Reiser[2], Joseph Vimal Vas[3], Thibaud Denneulin[3], Rafal E. Dunin-Borkowski[3], Patrick Maletinsky[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

This study investigates the origin of exchange bias in $Fe_3GeTe_2/MnPS_3$ vdW heterostructures. A substantial 170 mT exchange bias is observed at 5 K, one of the largest values reported for vdW heterostructures, despite the compensated interfacial spin configuration of $MnPS_3$. This exchange bias is linked to unexpected weak ferromagnetic ordering in $MnPS_3$ below 40 K that we reveal by NV center imaging. A 1000% variation in the magnitude of exchange bias is obtained through thermal cycling linked to changes in the vdW gap during field cooling. Detailed interface analysis reveals atom migration between layers, forming amorphous regions on either side of the vdW gap. These findings underscore the robust and tunable nature of exchange bias in vdW heterostructures but also challenge the often assumed pristine nature of vdW interfaces calling for in-depth interface characterization.

[1] A. P. Balan et al., Advanced Materials 36, 2403685 (2024).

HL 11: Ultra-fast Phenomena I

Time: Monday 16:00–18:45 Location: H14

HL 11.1 Mon 16:00 H14

Femtosecond Photocurrents in 2D materials — •Björn Sinz[1,2], Johannes Schmuck[1,2], Johannes Gröbmeyer[1,2], Nina Pettinger[1,2], Sergey Zherebtsov[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, TU Munich, Munich, Germany — [2]Munich Center of Quantum Science and Technology (MCQST), Munich, Germany

Light-field-driven currents have already been investigated in graphene by ultrashort laser pulses. In the strong-field regime, the electric field directly generates such photocurrents on a time scale of femtoseconds, whereas in the weak-field regime other photogeneration processes like the photo-thermoelectric effect dominate [1]. The different photocurrents are not limited to graphene but are also predicted for transition metal dichalcogenide (TMDC) monolayers. We report on femtosecond-pulse driven photocurrents in monolayer TMDC samples.

[1]: J. Gröbmeyer, P. Zimmermann, B. Huet, J. A. Robinson, A. W. Holleitner; Space-charge limited and ultrafast dynamics in graphene-based nano-gaps. Appl. Phys. Lett. 3 July 2023; 123 (1): 013504. https://doi.org/10.1063/5.0154152

HL 11.2 Mon 16:15 H14

Hot-Electron-Induced Substrate Response in Transient Absorption Spectroscopy of Tantalum — •Erik Willem de Vos[1,2], Sergej Neb[1], Marko Hollm[1], Florence Burri[1], Lukas Gallmann[1], and Ursula Keller[1] — [1]Department of Physics, Institute for Quantum Electronics, ETH Zurich, Switzerland — [2]Department of Materials, ETH Zurich, Zurich, Switzerland

We show that for extreme ultraviolet transient absorption spectroscopy measurements on thin-film metals, the substrate can significantly contribute to the observed change in absorption even if the substrate is transparent to the excitation wavelengths of the pump pulse and does by itself not produce a transient signal. Irradiation of a thin-film tantalum layer deposited on a silicon nitride substrate by a near-infrared femtosecond pulse is found to excite a coherent acoustic phonon in both the tantalum as well as the substrate. The response in the substrate rises on sub-picosecond timescales and is the result of direct excitation by the hot-electron distribution in the metal layer.

HL 11.3 Mon 16:30 H14

Nonequilibrium electron-phonon dynamics: dynamical control of quantum matter — •Yaxian Wang — Institute of Physics, Chinese Academy of Sciences

Electron-phonon interaction is an old yet evergreen problem in condensed matter physics. It is closely related to many quantum states we are concerned with, such as superconductivity, charge density waves, and polarons. It also profoundly affects, or often accompanies, critical phenomena such as the formation of excitonic insulators and metal-insulator transitions. When the system is driven out of equilibrium, for example pumped by an ultrafast laser pulse, the potential energy surface and thus the coupling in the excited states can be greatly reshaped, and this may open up a new avenue of ultrafast coherent control of quantum phases and topological orders. However, theoretical approaches often fail to capture the coupled dynamics of the non-thermal excited carriers and the nonequilibrium lattice order. In this talk, I will introduce how light-induced coherent phonons can cause a quasi-static lattice distortion and result in a Lifshitz transition in a nodal-line semimetal. We also demonstrate how the laser energy can shift the quasi-equilibrium lattice structure towards opposite directions, thus engineering the electronic structure via different regimes. Moreover, I will discuss our recent discovery on how nonequilibrium electron-phonon interaction can interact with the spin degree of freedom, causing ultrafast demagnetization and excitation of chiral phonons in a monolayer ferromagnet.

HL 11.4 Mon 16:45 H14

Nonequilibrium control of the ultrafast electron dynamics in semiconductors via light-driven coherent phonons — •Chenyu Wang[1,2], Yaxian Wang[1], and Sheng Meng[1,2,3] — [1]Institute of physics, Chinese Academy of Sciences — [2]School of physical sciences, University of Chinese Academy of Sciences — [3]Songshan Lake Materials Laboratory

Driving lattice vibration with a high degree of spatial and temporal coherence via strong light-matter interactions has emerged as a unique knob to control the out-of-equilibrium quantum states and the exotic ultrafast phenomena.

In this talk, I will present our recent theoretical works on the exploration and understanding of how the coherent phonon excitation can be utilized to control the electronic behaviors on ultrafast timescales, for example to engineer the carrier transport in monolayer WSe2 and to manipulate the nonrelativistic spin splitting in the prototypical altermagnetic semiconductor MnTe.

In photoexcited monolayer WSe2, we observe an unconventional 'step-like' electron intervalley scattering dynamics and meanwhile a Rabi oscillation driven by the coherent phonons, as a direct manifestation of the nonadiabatic electron-phonon coupling beyond equilibrium; On the other side, we demonstrate the light-driven coherent phonon can also be utilized to break the crystal symmetry in the altermagnet MnTe. Such symmetry breaking phase holds an extra spin-splitting particularly in the zone center, and thus a strongly enhanced spontaneous anomalous Hall effect.

HL 11.5 Mon 17:00 H14

Semiconductor Bloch Equations and Ehrenfest Dynamics in a Wannier Function Framework: An Integrated Approach to Ultrafast Electron and Ion Dynamics — •Stefano Mocatti, Giovanni Marini, Giulio Volpato, Pierluigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Real-time simulations of photoexcited semiconductors offer valuable insights but are challenged by the complex interplay of interactions and high computational cost. Here, we present an efficient ab initio scheme within the EPIq code, combining semiconductor Bloch equations with Ehrenfest dynamics in the Wannier representation. Electron-phonon and electron-electron interactions follow a Fan-Migdal+GW approximation, while phonon-phonon interactions include non-perturbative quantum anharmonic effects. Through the real-time tracking of the dynamics, we find that electron-electron interaction dominates photocarrier thermalization, yielding a double chemical potential electronic Fermi distribution. Furthermore, atomic forces converge to those calculated within constrained density functional perturbation theory. This work connects out-of-equilibrium and quasi-equilibrium states, advancing the understanding of ultrafast light-driven phenomena.

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15 min. break

HL 11.6 Mon 17:30 H14

Ultrafast Dynamic Coulomb Screening of X-ray Core Excitons in Photoexcited Semiconductors — •Thomas C. Rossi[1], Lu Qiao[2], Conner P. Dykstra[3], Ronaldo Rodrigues Pela[4], Richard Gnewkow[1,5], Rachel Wallick[3], John H. Burke[3], Erin Nicholas[3], Anne-Marie March[6], Gilles Doumy[6], D. Bruce Buchholz[7], Christiane Deparis[8], Jesus Zuñiga-Pérez[8,9], Michael Weise[10], Klaus Ellmer[10], Mattis Fondell[1], Claudia Draxl[2], and Renske M. van der Veen[1,5,11] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Department of Physics and CSMB, Humboldt Universität zu Berlin, Berlin, Germany — [3]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA — [4]Supercomputing Department, Zuse Institute Berlin (ZIB), Berlin, Germany — [5]Institute of Optics and Atomic Physics, Technische Universität Berlin, Berlin, Germany — [6]Chemical Sciences and Engineering Division, Argonne National Laboratories, Lemont, Illinois, USA — [7]Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States — [8]Université Côte d'Azur, CNRS, CRHEA, rue Bernard Gregory, Sophia Antipolis, Valbonne, France — [9]Majulab, International Research Centre Laboratory IRL 3654, Singapore — [10]Optotransmitter-Umweltschutz-Technologie (OUT) e.V., Berlin, Germany — [11]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA

The screening of core excitons is an inherent many-body process that can reveal insight into charge-transfer excitations and electronic correlations. Here we demonstrate the dynamic Coulomb screening induced by photoexcited carriers on core excitons employing X-ray transient absorption (XTA) spectroscopy with picosecond time resolution. Our interpretation is supported by state-of-the-art *ab initio* calculations including many-body perturbation theory. Using ZnO as an archetypal wide band-gap semiconductor, we show that the Coulomb screening modification at the Zn L_3- and K-edge leads to a decrease in the core-exciton binding energy. We also theoretically predict the effect of core-exciton screening on the femtosecond time scale for the case of ZnO, a major step towards hard X-ray excitonics. The results have implications for the interpretation of ultrafast X-ray spectra in general and their use in tracking charge carrier dynamics in complex materials on atomic length scales.

HL 11.7 Mon 17:45 H14

Ultrafast Coherent Dynamics of a Hybrid WS2/Plasmon Structure Probed by Two-Dimensional Electronic Spectroscopy — •Daniel Timmer[1], Moritz Gittinger[1], Daniel C. Lünemann[1], Thomas Quenzel[1], Sven Stephan[1,2], Martin Silies[1,2], Antonietta De Sio[1], and Christoph Lienau[1] — [1]IfP, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]ILO, Hochschule Emden/Leer, Emden, Germany

Transition metal dichalcogenide (TMD) monolayers (1L) have been established as important building blocks for quantum materials. Hybridization between light and matter states, in particular in plasmonic nanostructures, offers great opportunities to tailor their optical and electronic properties [1]. Here, we investigate such a hybrid plasmonic structure in the intermediate coupling regime comprised of 1L-WS2 [2] placed on a periodic silver nano-slit array using ultrafast two-dimensional electronic spectroscopy (2DES). We observe a 20-fold increase of the optical nonlinearity and ultrafast coherent plexciton dynamics during the dephasing time (~50 fs). We rationalize our observations via a Tavis-Cummings model that gives rise to collective dark states and a Rabi contraction of the 2-quantum states. Using ultrafast 2DES, we obtain access to probe and disentangle the coherent and incoherent dynamics in TMD-based plasmonic systems. [1]: Timmer et al. "Plasmon mediated coherent population oscillations in molecular aggregates." Nat. Commun. 14.1 (2023): 8035. [2]: Timmer et al. "Ultrafast Coherent Exciton Couplings and Many-Body Interactions in Monolayer WS2" Nano Lett. 24.26 (2024): 8117-8125.

HL 11.8 Mon 18:00 H14

Excited-state symmetry breaking and antisymmetric mode brightening in quadrupolar dye — •Somayeh Souri[1], Katrin WInte[1], Daniel Lünemann[1], Fulu Zheng[2], Mohamed Madjet[2], Teresa Kraus[3], Elena Mena-Osteritz[3], Peter Bäuerle[3], Sergei Tretiak[4], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Bremen University, Germany — [3]Ulm University, Germany — [4]Los Alamos National Laboratory, USA

Quadrupolar acceptor-donor-acceptor (A-D-A) dyes are chemically tunable materials displaying a rapid photo-induced charge transfer of interest for applications in solution-processed photovoltaics. The origin of the ultrafast charge transfer is unknown. Using sub-10-fs ultrafast spectroscopy, we investigate the excited-state dynamics of a prototypical A-D-A with comparable electronic and vibronic coupling strengths. Our results reveal that vibronic couplings to high-frequency C-C-stretching vibrations on each arm of the quadrupolar dye induce a double-minimum potential energy surface (PES) in the excited-state S1 driving symmetry breaking along the antisymmetric vibrational coordinate (Q-). Upon excitation, this induces periodic splitting of the optically launched coherent wavepacket along Q- with 20-fs period, rapidly relaxing into local minima of the symmetry-broken PES within less than 100 fs. Our results demonstrate highly nonadiabatic vibronic quantum dynamics, theoretically predicted for this class of dyes [1], and unravel their role for the ultrafast charge transfer in this class of molecules. [1] J. Chem. Phys. 141, 164317 (2014).

HL 11.9 Mon 18:15 H14

Phonon-driven exciton population oscillations in Methylammonium Lead Bromide Perovskites. — •Mohsin Sayar[1], Katrin Winte[1], Daniel Timmer[1], Somayeh Souri[1], Davide Ceratti[2], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Weizmann Institute of Science, Rehovot, Israel

Halide perovskites exhibit unique optoelectronic properties significantly influenced by electron-phonon interactions. Recent work shows that the internal fields induced by coherent lattice motions can transiently control ultrafast excitonic optical response in bulk $CsPbBr_3$[1]. Here, we demonstrate this behaviour also in $CH_3NH_3PbBr_3$ across different crystal phases, using temperature-dependent ultrafast transient reflectivity with 10 fs time resolution. Following resonant exciton excitation reveals coherent low-frequency phonon oscillations at 40cm^{-1} and 67cm^{-1}, corresponding to Pb-Br-Pb bending and stretching modes[2] that most strongly couple to the exciton. Additionally, we observe faster oscillations with dominant period of 105 fs in all crystal phases, arising from coherent exciton population transfer between 1s and 2p excitonic states, off-resonantly driven by the low-frequency phonon fields. We rationalize these results by a phenomenological model accounting for the coupling of excitons to the low frequency phonon modes and coupling of 1s-2p vibronic manifolds via the phonon fields[1]. These results may have important implications for transiently modifying the optoelectronic properties of perovskites.

HL 11.10 Mon 18:30 H14

Coherent suppression of high-harmonic generation in Dirac materials — •Wolfgang Hogger[1], Alexander Riedel[1], Debadrito Roz[2], Angelika Knothe[1], Cosimo Gorini[3], Juan-Diego Urbina[1], and Klaus Richter[1] — [1]Institute for theoretical physics, University of Regensburg, Germany — [2]Indian Institute of Science, Bengaluru 560012, India — [3]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

The study of high-harmonic generation in solids by intense laser pulses provides a fascinating platform for studying ultra-fast electron dynamics and material properties, where the coherent character of the electron dynamics is a central aspect. Starting with the semiconductor Bloch equations, we show the ubiquitous presence of a mechanism suppressing the high harmonic spectrum arising from the coherent superposition of intra- vs inter-band contributions to the total signal [1]. We provide evidence for the generality of this phenomenon by extensive numerical simulations exploring the parameter space of this coherent suppression of high harmonic generation in systems of massive Dirac Fermions (as a prototypical model for topologically non-trivial matter [2]), systems with a pseudo- relativistic dispersion. We supplement our numerical observations with analytical results for a simplified single-mode analysis.

[1] Y. Murakami and M. Sch*uler, Phys. Rev. B 106, 35204 (2022)
[2] C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Physical Review B 82, (2010)

HL 12: Quantum Transport and Quantum Hall Effects (joint session HL/TT)

Time: Monday 16:45–18:15 Location: H15

HL 12.1 Mon 16:45 H15

kdotpy: A Python application for k·p band structure simulations of zincblende semiconductors — •Wouter Beugeling[1,2], Florian Bayer[1,2], Christian Berger[1,2], Jan Böttcher[3], Leonid Bovkun[1,2], Christopher Fuchs[1,2], Maximilian Hofer[1,2], Saquib Shamim[1,2], Moritz Siebert[1,2], Li-Xian Wang[1,2], Ewelina M. Hankiewicz[3], Tobias Kiessling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik (TP4), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The software project kdotpy aims at simulations of electronic band structures of semiconductor devices with k·p theory. The application implements the widely used Kane model, capable of reliable predictions of transport and optical properties for a large variety of topological and non-topological materials with a zincblende crystal structure.

In this presentation, I present the core functionality and features of kdotpy. I will explain how we have implemented principles of modern software engineering and good scientific practice in this project.

HL 12.2 Mon 17:00 H15

End states in zigzag Haldane model nanoribbons — Simone Traverso, Maura Sassetti, and •Niccolò Traverso Ziani — Physics Department, University of Genova, Italy

As topological materials based on the graphene lattice become experimentally realizable in materials such as germanene, the physics of the bound states that characterize them at step edges and in quasi one-dimensional settings becomes relevant.

In this context, the appearance of topological bound states in zigzag Haldane nanoribbons will be addressed [1]. A reentrant topological phase diagram is found. Together with numerical results, a low energy theory extending the Jackiw-Rebbi paradigm will be presented.

[1] S. Traverso, M.Sassetti, N. Traverso Ziani, NPJ Quantum Materials 9, 9 (2024).

HL 12.3 Mon 17:15 H15

Time-reversal invariant Chalker-Coddington model and the real-space renormalisation group — •Syl Shaw and Rudolf A. Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

The Chalker-Coddington model has been utilised to great success in understanding the plateau transitions in the quantum Hall effect. Since the model's inception, it has been extended to a time-reversal invariant symmetry class to describe the quantum-spin Hall effect. Here we adapt a real-space renormalisation group method[1] to respect time-reversal symmetry and use it investigate the phase diagram of the quantum-spin Hall effect. We aim to find distinct phases as a function of both saddle-point height, z and spin-mixing angle ϕ. At the phase boundary between insulator and metal, we compute the value of the critical exponent of the localisation length, ν, with the same real-space renormalisation technique. [1] S. Shaw, R. A. Römer Physica E 165, 116073 (2025)

HL 12.4 Mon 17:30 H15

Utilizing Silicon Qubit Devices for Quantum Electrical Metrology — •Dustin Wittbrodt[1], Johannes Christian Bayer[1], Lars Schreiber[2,3], Janne Lehtinen[4], Marcelo Jaime[1], and Frank Hohls[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Forschungszentrum Juelich, Juelich, Germany — [4]SemiQon Technologies Oy, Espoo, Finland

The 2019 redefinition of the SI system established fixed values for fundamental constants such as the elementary charge (e) and the Planck constant (h), enabling the quantum realization of the units of Ampere, Volt, and Ohm. While the quantum realization of Volt and Ohm is well-established, the realization of the Ampere, whether directly through Single Electron Pumps (SEPs) or indirectly via the Volt and Ohm, has yet to achieve the same level of accuracy. Moreover, further device applications in practical circuits require paralelization approaches to achieve higher current outputs. The international project "Advanced Quantum Technology for Metrology of Electrical Currents" (AQuanTEC) aims to upscale SEPs beyond the 1 nA threshold. To achieve this, AQuanTEC explores several strategies, including the use of silicon devices first designed for spin qubit realization. These devices are highly promising due to their potential scalability, driven by ongoing advancements in integrating large numbers of qubits.

HL 12.5 Mon 17:45 H15

Surface state dominated transport in HgTe topological insulator devices — •Maximilian Hofer[1,2], Christopher Fuchs[1,2], Lena Fürst[1,2], Tobias Kiessling[1,2], Wouter Beugeling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

Recently grown three dimensional topological insulators based on tensile strained HgTe exhibit an exceptionally high mobility and very low intrinsic carrier density. The high quality material has made it possible to study the Landau level dispersion at low magnetic fields and identify four distinct transport regimes. We demonstrate that while a contribution from the topological surface states to transport measurements is expected across the full experimentally accessible density range, there exists only a narrow density regime for which the electronic transport is exclusively carried by the topological surface states. We present the corresponding phase diagram for pure topological surface state transport depending on layer thickness and carrier concentration. For thick HgTe films grown pseudomorphically strained on CdTe, the total carrier density needs to be kept between $1.8 \times 10^{11}\,\mathrm{cm}^{-2}$ and $2.6 \times 10^{11}\,\mathrm{cm}^{-2}$ to remain in the pure surface state region and avoid contributions from bulk states. The experimental observations are supported by eight band $\boldsymbol{k} \cdot \boldsymbol{p}$ band structure calculations.

HL 12.6 Mon 18:00 H15

Designing a quantum sorter based on two-dimensional topological insulators — •Amanda Teodora Preda[1,2], Iulia Ghiu[2], Lucian Ion[2], Andrei Manolescu[3], and George Alexandru Nemnes[1,2] — [1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, Magurele- Ilfov, 077125, Romania — [2]University of Bucharest, Faculty of Physics, Atomistilor 405, Magurele-Ilfov, 077125, Romania — [3]Department of Engineering, Reykjavik University, Menntavegur 1, Reykjavik IS-102, Iceland

The idea of a quantum sorter emerged in quantum information, a field that aims to exploit quantum effects and manipulate qubits for information processing. In theory, it was proven that one can propose a universal quantum sorter for any arbitrary observable. To this point, suitable experimental schemes of implementation for this proposal were explored mainly in quantum optics. In our study, we introduce a solid-state version of a quantum sorter, based on a multi-terminal mesoscopic device with multiple output ports, that aims to separate the incoming states by both their spin and transversal mode. In order to maximize the state-separation efficiency of such a device, we chose to exploit the unique transport properties of topological insulators. Employing the tight-binding based simulation package Kwant, we modeled a device that meets the criteria of an irreversible quantum sorter, using the well-established BHZ Hamiltonian to simulate a multi-terminal quantum system made up of both trivial and topological materials.

HL 13: Heterostructures, Interfaces and Surfaces

Time: Monday 16:45–18:30 Location: H17

HL 13.1 Mon 16:45 H17

reducing waste through substrate reuse: a pathway to cost-effective iii-v optoelectronics — •Radouane Ennadir — 3IT, Sherbrooke University, Sherbrooke, QC, Canada

III-V materials, such as Gallium Arsenide (GaAs), are widely used in optoelectronic devices due to their superior electronic and optical properties. However, the high cost of III-V substrates, primarily made from Ge or other expensive materials, represents a significant barrier to the widespread adoption of these technologies. Our research focuses on reducing waste in the production of III-V optoelectronics through the reuse of Germanium (Ge) substrates. In this study, we propose a novel approach to mitigate substrate waste by reusing Ge substrates in the fabrication of III-V optoelectronics. By carefully optimizing the recycling process, including substrate cleaning, surface treatment, and the integration of new III-V layers, we aim to significantly reduce material costs without compromising device performance. This approach not only enhances the sustainability of optoelectronic manufacturing but also provides a cost-effective pathway to large-scale production of III-V-based devices. The findings of this study contribute to both environmental sustainability and economic viability in the growing field of optoelectronics, opening up new opportunities for the development of advanced, cost-effective optoelectronic devices.

HL 13.2 Mon 17:00 H17

Understanding local charge transfer processes in nanostructured photosystems — •Nina Miller, Sven Doll, Sergej Levashov, Lukas Wolz, Matthias Kuhl, and Johanna Eichhorn — Physics Department, School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical energy conversion offers a promising approach for directly converting solar energy into storable chemical fuels. For scalability, photoelectrodes are often fabricated using thin film technologies yielding material architectures with complex micro- and nanoscale structures. One challenge in this context is that the characteristics of these nanostructured material architectures often deviate from the properties of idealized model systems. To understand energy conversion processes at surfaces and interfaces of nanostructured material systems, novel atomic force microscopy methods have emerged recently, such as AFM-based scanning electrochemical microscopy, to resolve local chemical transformations, charge transport, and material changes under operation conditions. By correlating nanoscale and macroscale properties, we will establish the link between nanoscale processes and macroscopic performance, advancing the design of efficient semiconductor/catalyst systems for PEC applications.

HL 13.3 Mon 17:15 H17

Simulation of charge and excitation dynamics across nanostructured organic-organic interfaces — •Giacomo Cotelli[1,2], Engin Torun[2], Stefano Gottardi[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics (EP II), University of Bayreuth, Bayreuth 95440, Germany — [2]Simbeyond B.V., Eindhoven, The Netherlands

The deposition of organic layers via solution processing may lead to rough interfaces or intermixed regions between layers. To investigate the impact of roughness at organic-organic interfaces on the performances of OLEDs, we performed 3D kinetic Monte Carlo simulations of symmetrical bi- and three-layer devices. Our results reveal that the macroscopic behaviour of a device can be significantly affected by the shape and size of roughness at the organic interfaces, influencing both charge and exciton dynamics.

Namely, we introduced interfaces with periodic corrugation and either triangular or rectangular cross-section. In presence of charge accumulation at an interface with triangular cross-section, bilayer devices exhibit strong inhomogeneity in the spatial distribution of charge carriers, excitons and excitonic losses. Comparison to a flat-interface device reveals an increment in current density by a factor from 2 to 10^3, depending on the height of the energy barrier at the interface. This current density boost was successfully applied to improve charge injection towards a central emissive layer (EML) in simulated three-layer devices; the size and configuration of the interfaces can also be leveraged to fine-tune the recombination zone inside the EML. Nevertheless, we raise our concerns in terms of increased local material degradation.

HL 13.4 Mon 17:30 H17

Strain gradients in bent GaAs nanowires as a new way of engineering electronic transitions — •Francisca Marín[1], Yiannis Hadjimichael[2], Christian Merdon[2], Patricio Farrell[2], Constanza Manganelli[3], Oliver Brandt[1], and Lutz Geelhaar[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V. Berlin, Germany — [2]Weierstraß-Institut für angewandte Analysis und Stochastik. Berlin, Germany — [3]Institut für Halbleiterphysik, Leibniz-Institut für innovative Mikroelektronik. Frankfurt (Oder), Germany

Strain gradients open up a new degree of freedom in strain engineering, enabling polarization in all dielectric materials through the flexoelectric effect. However, flexoelectric coefficients remain unknown for many inorganic semiconductors, including GaAs, leaving this phenomenon unexplored in this material system.

Here, we exploit the pronounced strain gradient in bent GaAs nanowires grown by molecular beam epitaxy to study this effect using photoluminescence spectroscopy. Strain and strain gradients in these nanowires influence the bandgap and generate electric fields from piezoelectric and flexoelectric effects. By combining experiments with a simple one-dimensional model to calculate the expected shift of the electronic transitions, and finite element simulations of piezoelectricity, we provide new insights into flexoelectricity in GaAs.

HL 13.5 Mon 17:45 H17

Understanding Local Charge Transport Using Advanced Kelvin Probe Force Microscopy — •Sven Erik Doll, Sergej Levashov, Nina Miller, and Johanna Eichhorn — Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.

To this end, we use Kelvin probe force microscopy (KPFM) in a controlled atmosphere to spatially resolve band bending, charge accumulation, and local variations of the generated surface photovoltage. However, analyzing nanostructured materials with complex morphologies is not trivial since topographic crosstalk can dominate the results. To overcome these limitations, we combine a commercial AFM with an external Lock-In amplifier to enable dual-frequency and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventionally frequency-modulated and amplitude-modulated KPFM modes. Here, we compare different KPFM modes and highlight the importance of careful imaging and data analysis to reveal insights into local semiconductor material properties at grain boundaries or different facets.

HL 13.6 Mon 18:00 H17

Topological Phase Diagram of Mercury Cadmium Telluride Quantum Wells — •Leonid Bovkun[1,2], Lena Fürst[1,2], Christopher Fuchs[1,2], Vladimir Marković[1,2], Maximilian Hofer[1,2], Moritz Siebert[1,2], Christian Berger[1,2], Florian Bayer[1,2], Wouter Beugeling[1,2], Steffen Schreyeck[1,2], Hartmut Buhmann[1,2], Laurens W. Molenkamp[1,2], and Tobias Kiessling[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

The key ingredient for the formation of a topological insulator phase in Mercury Cadmium Telluride is the inversion of the energetic positions of the electronic Γ_6 and Γ_8 bulk bands, that can be controlled by alloying with Cd to get within reach of electronic tunability.

We present a systematic experimental study of the topological phase transition in a series of $\sim$10 nm thick $Hg_{1-x}Cd_xTe$ quantum wells by tuning the Cd content x. We provide detailed structural and magneto-optical spectroscopic characterization measurements and establish a comprehensive picture of the alloy structural and energetic properties.

Using these as input, we employ $\mathbf{k}\cdot\mathbf{p}$ modeling to establish the topological phase diagram of $Hg_{1-x}Cd_xTe$ in dependence of the Cd content and quantum well thickness for thin films which are pseudomorphically

strained to the lattice constant of pure CdTe.

HL 13.7 Mon 18:15 H17

Electrostatic control of the band structure in HgTe heterostructures — •Moritz Siebert[1,2], Maximilian Hofer[1,2], Leonid Bovkun[1,2], Vladimir Marković[1,2], Christian Berger[1,2], Florian Bayer[1,2], Julian Kuther[1,2], Daniel Michel[1,2], Lena Fürst[1,2], Christopher Fuchs[1,2], Wouter Beugeling[1,2], Steffen Schreyeck[1,2], Hartmut Buhmann[1,2], Laurens W. Molenkamp[1,2], and Tobias Kiessling[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

We investigate the band structure of topologically inverted thick HgTe quantum wells employing magneto-optical THz- and IR-spectroscopy. The lithographic fabrication of a semi-transparent gate enables control of the charge carrier density in the quantum well. Our magnetic field dependent self-consistent $\mathbf{k} \cdot \mathbf{p}$ band structure calculations give insights into the physical origin of the observed spectral signatures. In this talk, I present how the electrostatic gating not only sets the number of free charge carriers in the HgTe quantum well - but also modifies the electronic dispersion - and explain the observed features.

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

Time: Tuesday 9:30–13:00 Location: H3

Invited Talk HL 14.1 Tue 9:30 H3

Graphene-based epitaxial 2D heterosystems: making graphene great again — •Christoph Tegenkamp — Institut für Physik, TU Chemnitz

2D materials and their heterostructures are at the forefront of research, anticipated to serve as fundamental building blocks for new quantum materials. Proximity coupling is a key concept in this domain, enabling diverse and novel functionalities. Epitaxial graphene (EG) grown on SiC(0001) resembles a truly 2D electron gas system, celebrated for its manifold and flexible functionalization schemes at both its vacuum and interface sites. These functionalization strategies enable extreme doping scenarios in graphene, tuning spin-orbit coupling, realizing interface states, or introducing mini-bands through zone folding. The controlled transition from linear to flat bands in EG, along with the coupling of functionalized epitaxial graphene to 2D electron gases (2DEGs), opens avenues for exploring electronic correlation effects and mesoscopic phenomena in epitaxial 2D heterostructures. In this presentation, I will showcase some recent findings achieved through the adsorption and intercalation of elements such as Pb and Sn, demonstrating their potential to further tune the properties of graphene.

HL 14.2 Tue 10:00 H3

Proximity-induced spin-orbit coupling in bilayer graphene quantum wires — •Michael Laumer and Angelika Knothe — Universität Regensburg, 93053 Regensburg, Germany

The gate-tuneable band gap and the possibility to tailor its band structure by proximitizing with other 2D materials [1] make bilayer graphene (BLG) an excellent platform for future quantum technologies. By applying spatially modulated displacement fields, one may confine BLG's charge carriers into electrostatically induced nanostructures [2, 3]. Proximitizing the BLG with a transition metal dichalcogenide (TMDC) strongly enhances the SOC of the adjoining graphene layer [1]. Fascinated by the concept of proximity-tailoring BLG nanostructures, we convey the idea of proximity-inducing SOC to a gate-confined BLG quantum wire. We theoretically study the resulting quantized subband structure for different SOC strengths and as a function of the wire geometry. Our results help us understand how proximity-induced SOC manifests in confined geometries and identify different regimes of the wires' electronic properties.

[1] K. Zollner, M. Gmitra, and J. Fabian. Swapping exchange and spin-orbit coupling in 2d van der waals heterostructures. Phys. Rev. Lett., 125:196402, (2020). [2] A. Knothe and V. Fal'ko. Influence of minivalleys and berry curvature on electrostatically induced quantum wires in gapped bilayer graphene. Phys. Rev. B, 98:155435, (2018). [3] H. Overweg et al. Topologically nontrivial valley states in bilayer graphene quantum point contacts. Phys. Rev. Lett., 121:257702, (2018).

HL 14.3 Tue 10:15 H3

Above room temperature ferromagnetism in large-area Fe_3GaTe_2/graphene van der Waals heterostructures — •Tauqir Shinwari[1], Kacho Imtiyaz Ali Khan[1], Hua Lv[1], Atekelta Abebe Kassa[1], Frans Munnik[2], Achim Trampert[1], Michael Hanke[1], Jens Herfort[1], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V. Dresden, Germany

Two-dimensional (2D) magnetic materials and van der Waals (vdW) heterostructures offer new possibilities for the realization of advanced spintronic devices. Fe_3GaTe_2, a 2D ferromagnetic metal with a high Curie temperature ($\sim$ 360K) and strong perpendicular magnetic anisotropy, has emerged as a promising candidate for energy-efficient magnetic devices. However, all investigations conducted in Fe_3GaTe_2 so far have been performed using millimeter-sized bulk crystals and flakes exfoliated from them, both not suitable for integration in device processing. Hence, it is crucial to develop controlled large-scale growth of this material and investigate its properties. In this contribution, we present a breakthrough in the high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films on epitaxial graphene/SiC(0001) substrates using molecular beam epitaxy. These results are highly relevant for the future development of high-performance spintronic devices based on 2D heterostructures potentially revolutionizing data storage, processing, and quantum computing applications.

HL 14.4 Tue 10:30 H3

Modeling carbon nanomembranes through molecular dynamics simulations — •Levin Mihlan and Jürgen Schnack — University of Bielefeld

Carbon nanomembranes (CNMs) are nanometer-thin materials synthesized via electron-induced crosslinking of aromatic self-assembled monolayers. CNMs can be functionalized for various applications, initially serving as molecular filters. Due to their presumed irregular internal structure, these membranes pose challenges for standard spectroscopic efforts, often being insufficiently informative [1]. Ehrens et al. initially conducted molecular dynamics simulations to investigate CNM formation, replicating crosslinking and pore formation via momentum transfers in carbon-only systems [2]. Here, we extend the approach by incorporating hydrogen atoms, which may play a critical role in the crosslinking process, even though they largely disappear in the final CNM products. This additionally reduces the number of theoretical assumptions. We examine whether and in what way pores form and analyze properties such as aromaticity, sp content, and Young's modulus to compare with previous simulations and experiments.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" Chem. Phys. Chem 21, 1006 (2020)
[2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416 (2021)

session break

HL 14.5 Tue 11:00 H3

Photo-electrochemical oxidation and thinning of transition metal dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Franz Gröbmeyer[2], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Walter Schottky Institute, Physics Department and TUM School of Natural Science, Technical University of Munich — [2]Nanoinstitute Munich and Faculty of Physics, Ludwig-Maximilians-Universität — [3]Naval Research Laboratory, Washington, D.C

Two-dimensional transition metal dichalcogenides (TMDs) exhibit unique optoelectronic and mechanical properties. For their integration in functional devices and for catalytic applications, it is crucial to understand and control their behavior in the reactive environments. Here, we investigate the stability of thin MoS_2, WS_2, $MoSe_2$ and WSe_2 films in acidic, neutral, and basic solutions using a three-electrode photoelectrochemical cell, which enables experiments under both illumi-

nation and in the dark. Under anodic conditions, sulfides and selenides undergo different protonic reactions, depending on the pH of the electrolyte, resulting in different resistances to oxidation. Additional exposure to light from a solar simulator creates photo-excited holes, which drive a self-limiting electrochemical thinning procedure that enables the top-down fabrication of large-area TMDs with a thickness of only a few layers. The degradation, initiated at the edges or defects, propagates through the flakes and can be monitored in-situ using an optical microscope. Under laser excitation, multilayer TMDs can be thinned in predefined patterns, paving a new route for processing and integration of 2D materials into functional devices.

HL 14.6 Tue 11:15 H3

Rapid MOCVD synthesis of stratified MoS2 and WS2 2D heterostructures — •Nikolas Dominik, Sebastian Klenk, Cormac Ó Coileáin, and Georg S. Duesberg — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, München, Deutschland

The two-dimensional (2D) structure of layered materials such as the transition metal dichalcogenides MoS2 and WS2, imparts exceptional electrical, mechanical and optical properties. This makes them particularly interesting for electronic, photovoltaic and sensing application. Van der Waals heterostacks, composed of assembled 2D materials, expand on the possible range of properties, and so have attracted extensive attention due to factors such as ultrafast carrier transport and high bandgap tunability.

Here we present metal-organic chemical vapour deposition (MOCVD) synthesis of MoS2/WS2 combination heterostructures using a highly controllable industrial-scale multi-precursor system, thus avoiding the laborious need for manual stacking. We show how this synthesis method allows the creation of clearly defined and highly ordered stacks by producing a 7-layer combination structure below 10 nm. We explore the characteristics of these films using Raman spectroscopy and XPS, EDX, TOF-SIMS and microscopy techniques.

HL 14.7 Tue 11:30 H3

Unveiling the mechanism of monolayer selective large-area exfoliation of 2D materials — •Jakob Ziewer[1], Abyay Ghosh[1], Michaela Hanušová[2], Luka Pirker[2], Otakar Frank[2], Matěj Velický[2], Myrta Grüning[1], and Fumin Huang[1] — [1]Queen's University Belfast, Belfast, U.K. — [2]J. Heyrovský Institute of Physical Chemistry

Metal assisted exfoliation has made it possible to selectively isolate single crystal monolayers of 2D materials at sizes up to a centimetre [1][2]. This represents a million fold increase compared to standard tape exfoliation.

In this presentation the mechanism of enhanced yield is discussed. Through spectroscopic measurements and observation of macroscopic bubbles it is discovered that the Au substrate decouples attached MoS_2 monolayers from the remaining crystal. The interfacial weakening is dependant on the thickness of the crystal and is maximised for thick crystals.

These findings are used to explain the mechanism behind metal assisted exfoliation and are expected to extend to other Au-2D heterostructures.

[1] Velický, M.; et. al. Mechanism of Gold-Assisted Exfoliation of Centimeter-Sized Transition-Metal Dichalcogenide Monolayers. ACS Nano 2018, 12, 10463*10472. [2] Huang, Y.; et. al. Universal Mechanical Exfoliation of Large-Area 2D Crystals. Nat. Commun. 2020, 11:2453.

session break

HL 14.8 Tue 12:00 H3

Probing the electronic band structure of the 2D magnetic materials MPS3 (M=Fe,Ni) across magnetic phase transitions — •Jeff Strasdas[1], Benjamin Pestka[1], Biplab Bhattacharyya[1], Adam K. Budniak[2], Marcus Liebmann[1], Niklas Leuth[1], Honey Boban[3], Lutz Waldecker[1], Bernd Beschoten[1], Christoph Stampfer[1], Lukasz Plucinski[3], Efrat Lifshitz[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH, Aachen, Germany — [2]Schulich Chem. Fac., Solid State Inst., Russell Berrie Nanotech. Inst., Helen Diller Quantum Center, Technion - Israel Inst. of Technology, Haifa, Israel — [3]Forschungszentrum Jülich, Peter Grünberg Inst. (PGI-6), Jülich, Germany

We investigate the band structure of the van der Waals materials FePS3 [1] and NiPS3, both 2D antiferromagnetic insulators, using μm-scale Angular Resolved Photoelectron Spectroscopy (ARPES), above and below their Néel temperatures (TN). The data is compared with DFT+U calculations and simplified selection rules to deduce the orbital character of changing bands. In FePS3, we observe three distinct band structure changes across TN, involving bands with Fe 3d, S 3p, and pure P 3p character, reflecting the intricate competition of direct exchange between Fe atoms and superexchange via S and P atoms. In NiPS3, we identify one band shift near Γ across TN, containing a band of mixed Ni and S character. Here, pronounced deviations from the DFT+U calculations indicate more complex electronic correlations. Moreover, we refine the photoelectron selection rules using ARPES data from CrPS4. [1] B. Pestka et al. doi:10.1021/acsnano.4c12520

HL 14.9 Tue 12:15 H3

Investigation of 1T-TaS2 phase transition and charge transfer phenomena at interfaces with perovskites — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Centre of Scientific Research Demokritos, 15341 Athens, Greece — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Athens, Greece

1T-TaS2 is a distinguished 2D-layered transition metal dichalcogenide with a rich phase diagram upon cooling including charge density wave (CDW) states and a Mott insulating phase. On the other hand, halide perovskites (HPs) are emerging as a unique class of materials in the field of photonics due to their intriguing optoelectronic properties. The combination of 1T-TaS2 with HPs is proposed as a viable solution to overcome the drawbacks of each category thanks to charge transfer phenomena.

In this work, we studied the phase transitions of 1T-TaS2 as a function of the cooling rate. In the case of nanothick crystals, CDW phase transitions were observed upon gradual cooling but they were totally absent afrer a vigorous cooling. On the contrary, for bulk crystals the CDW phase transitions were totally independent of the cooling rate. Furthermore, we developed 1T-TaS2/HPs heterostructures and we investigated charge transfer phenomena by XPS and UPS spectroscopy, both revealing electron transfer from 1T-TaS2 towards perovskite. Charge transfer could also enable the development of high-performance hybrid optoelectronic devices based on these materials.

HL 14.10 Tue 12:30 H3

The effect of a perpendicular electric field on charge-spin interconversion coefficients in proximitized graphene on 1T-TaS_2 monolayer — •Juraj Mnich[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

The proximity-induced spin-orbit coupling and exchange interactions in the graphene-based heterostructures provides an effective way to manipulate with charge-spin interconversion coefficients. In the talk we focused on charge-spin interconversion in bilayer and trilayer heterostructures of 1T-TaS_2 and graphene. By modulating the temperature, we can access the charge density wave phase and switch between the magnetic and non-magnetic phases of 1T-TaS_2 affecting consequently the graphene electrons. Using linear response theory we showed the dependence of charge-spin interconversion coefficients on a perpendicular applied electric field. For the specific configurations of the 1T-TaS_2 and graphene we observed a change in both the sign and the magnitude of the non-equilibrium spin density as a response to the perpendicular electric field. This result indicates a possibility of using electric fields as a tool to control the direction of spin density.

This work was supported by the APVV-SK-CZ-RD-21-0114 and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008.

HL 14.11 Tue 12:45 H3

Self spin-orbit torque in proximitized graphene on 1T-TaS_2 monolayer — •Martin Gmitra[1,4], Maedeh Rassekh[1], Juraj Mnich[1], and Marko Milivojević[2,3] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

We show that self spin-orbit torque induced in graphene-based van der

Waals heterostructures represents a platform to extract the Rashba phase – a proximity-induced spin-orbit coupling parameter. Performing first-principles calculations, tight-binding modeling, and non-equilibrium Greens function transport calculations for graphene on 1T-TaS_2 monolayer we found that charge current in graphene generates non-equilibrium spin accumulation and self-torque in graphene due to the proximity-induced spin-orbit coupling and exchange interaction. The Rashba spin-orbit torque is a dominant contribution and weakly depends on the direction of magnetization in 1T-TaS_2. We propose that the magneto-optical Kerr effect can directly extract the Rashba spin-orbit coupling phase.

This work was supported by the APVV-SK-CZ-RD-21-0114, EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008, and IMPULZ IM-2021-42.

HL 15: Quantum Dots and Wires: Growth and Properties

Time: Tuesday 9:30–11:00 Location: H13

HL 15.1 Tue 9:30 H13

Predictive theory of multi-particle states of GaAs quantum dots — •Petr Klenovsky — Masaryk University, Brno, Czech Republic — Czech Metrology Institute, Brno, Czech Republic

The correlated multi-particle electronic structure of GaAs quantum dots (QDs) in AlGaAs matrix is studied. GaAs QDs have unique physical properties, like an absence of built in strain as well as exhibiting the effects of the weak confinement, leading to the superradiance. GaAs QDs are an almost ideal candidate as a source of single and entangled photons for usage in quantum cryptography and computing. Unfortunately, so far current physics models of their electronic structure were not successful to *quantitatively* reproduce observed experimental results like, e.g., binding energies of trions (X+ and X-) and biexciton (XX) with respect to exciton (X) as well as the radiative emission of those complexes. We endeavored to change that and show in this contribution the results of our improved theory model based on **k·p** approximation and configuration interaction (CI) schemes. Using that we demonstrate computed binding energies of X+, X-, and XX in agreement with experiment which are also *converged* with respect to the size of CI basis, i.e., they include the effects of the Coulomb correlation. While the latter is found to be of a paramount role, surprisingly, we also find that the binding energies strongly depend on the way the electron-electron and hole-hole *exchange* integrals are calculated. Our results show very good agreement with photoluminescence and nuclear spin relaxation experiments on GaAs/AlGaAs QDs.

HL 15.2 Tue 9:45 H13

Electron capture and emission dynamics of self-assembled quantum dots far from equilibrium — •Maximilian Erdmann[1], Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Severin Krüger[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

The subject of the experiment were the electron capture and emission dynamics of Self-Assembled Quantum Dots (SAQD) far away from equilibrium conditions, at a temperature of 77 K. The SAQDs are located in a semiconductor structure that can be regarded as a Schottky diode. For analysing the capture and emission dynamics, the capacitance transients of this sample were investigated using the methods of Deep Level Transient Spectroscopy (DLTS).

HL 15.3 Tue 10:00 H13

Spatial Statistics of InAs Quantum Dots on GaAs(100) — •Normen Auler[1], Viktoryia Zolatanosha[2], and Dirk Reuter[1,2,3] — [1]Department Physik, Universität Paderborn, DE — [2]Institute for Photonic Quantum Systems (PhoQS), Universität Paderborn, DE — [3]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, DE

Self-assembled InAs quantum dots (QDs) on GaAs are potential building blocks for quantum technology applications. One interesting aspect is the spatial arrangement of the QDs.

In this contribution, we investigated the spatial distribution of QDs for samples with different QD densities by analyzing atomic force microscopy images. We evaluated Voronoi cell areas and nearest neighbor configurations. Contrary to the expected random distribution for Stranski-Krastanow-grown QDs, we observe deviations indicating an influence of strain fields and a corresponding effect on inter-island adatom diffusion on the final QD arrangement. We discuss the behavior for different densities in detail.

HL 15.4 Tue 10:15 H13

Epitaxial growth and in-situ integration of high-quality single InGaAs quantum dots on a silicon substrate — •Imad Limame[1], Peter Ludewig[2], Aris Koulas-Simos[1], Chirag C. Palekar[1], Wolfgang Stolz[2], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin — [2]NAsP III/V GmbH, Marburg, Deutschland

For over two decades, the integration of light sources onto the silicon (Si) platform has garnered significant interest in both scientific and industrial communities. Despite the cost-effectiveness of Si and its extensive use in semiconductor technology, its indirect bandgap limits its potential for optoelectronic applications. The direct growth of III-V materials, which offer excellent optical properties, on Si is appealing but challenging due to factors such as lattice mismatch, differences in thermal expansion coefficients, Si surface reactivity, and dislocation formation. We report on the direct epitaxial growth of InGaAs QDs in both the 940 and 1300 nm ranges with excellent quantum optical properties on a Si substrate. The heteroepitaxy of GaAs heterostructures on Si is achieved using a GaP buffer layer. The resulting QDs exhibit outstanding optical properties, showcasing the significant potential of this approach. Furthermore, using a strain-reducing layer (SRL), we grow single QDs in the telecom O-band, which are then integrated via in-situ electron beam lithography (EBL) into circular Bragg gratings (CBG) to enhance extraction efficiency for quantum communication applications.

Our results represent a significant step toward scalable, cost-effective, and Si-compatible quantum photonics devices.

HL 15.5 Tue 10:30 H13

Electrostatic Inter-Layer Coupling between Self-Assembled Quantum Dots — •Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Charlotte Rothfuchs-Engels[2], Nikolai Bart[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

Electrostatic coupling between Self-Assembled Quantum Dots (SAQDs) in spatially separated layers is studied using transient capacitance spectroscopy. The coupling effect is analysed as a function of temperature, applied bias voltage, and the occupancy of the quantum dot layers. The observed interaction is attributed to the electric field modulation induced by charge redistribution in one layer, influencing the capture and emission dynamics in the other. A rate equation model was developed, incorporating self-consistent band bending calculations, to describe the impact of the inter-layer coupling on the charge transfer processes. The findings indicate that the coupling arises from the electrostatic field generated by the charged quantum dots in the adjacent layer, providing a quantitative explanation for the altered capacitance transients.

HL 15.6 Tue 10:45 H13

Photoluminescence from SiGe and Ge quantum dots on Si nanotips: role of composition and capping — •Diana Ryzhak[1], Johannes Aberl[2], Enrique Prado-Navarrete[2], Lada Vukušić[2], Agnieszka Anna Corley-Wiciak[1], Oliver Skibitzki[1], Marvin Hartwig Zoellner[1], Markus Andreas Schubert[1], Michele Virgilio[3], Moritz Brehm[2], Giovanni Capellini[1,4], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenberger Strasse 69, 4040, Linz, Austria — [3]Dipartimento di Fisica E. Fermi, Università di Pisa, Largo Pontecorvo 3, 56127, Pisa, Italy — [4]Dipartimento di Scienze, Università Roma Tre, V.le G. Marconi 446, 00146 Roma, Italy

Quantum dots (QDs) have been studied for their unique optical properties, which are essential for LEDs and lasers. The main challenge remains to control the fabrication processes of QDs. Therefore, we have used a nanoheteroepitaxy (NHE) approach and fabricated nearly strain-free SiGe and Ge QDs on Si(001) nanotip (NT) patterned substrates. The QDs were deposited by molecular beam epitaxy at 850°C, yielding defect-free structures selectively on the NTs as observed by transmission electron microscopy. Upon tuning the Si content, the photoluminescence (PL) peak emission shifted from 0.78 to 0.9 eV. The PL emission can be remarkably enhanced by capping the QDs with Al2O3 or Si3N4 for reduction of the surface recombination processes.

HL 16: Organic Semiconductors

Time: Tuesday 9:30–12:00 Location: H14

HL 16.1 Tue 9:30 H14

Modeling charge transport in organic semiconductors: why and when the conventional Miller-Abrahams rate is inappropriate — •Magdalena Dörfler, Heinz Bässler, Andrey Kadashchuk, Harald Oberhofer, and Anna Köhler — Universität Bayreuth, 95447 Bayreuth

A widely applied expression to model charge transport in organic semiconductors is the Miller-Abrahams rate, which describes the probability for charge transfer from one site, e.g. a molecule, to a neighboring site. However, the expression that is conventionally referred to as Miller-Abrahams rate is an approximation of a more general term. This approximation is only valid when energy differences between neighboring sites are large compared to the thermal energy. Here, we show the differences that result when charge transport is modelled by kinetic Monte Carlo simulations (KMC) using either of the two expressions. The widely used, approximate, rate can lead to serious errors in the magnitude and, more importantly, in the trends obtained for the temperature and field dependence of charge transport. The implications for modelling work and the interpretation of experimental data are discussed.

HL 16.2 Tue 9:45 H14

Accurate ab-initio parametrization of electron-phonon coupling models with Gaussian and plane-wave basis sets — •Konrad Merkel[1], Maximilian Dorfner[1], Manuel Engel[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, TU Munich, Germany — [2]VASP Software GmbH, Vienna, Austria

For the simultaneous treatment of electronic and vibrational degrees of freedom, the Holstein-Peierls model has become a cornerstone in various scientific communities due to its versatility and remarkable success in the accurate description of materials. To use it, one needs to calculate all model parameters for the electronic structure, phonons and electron-phonon coupling constants. In particular, the calculation of the electron-phonon coupling constants is a challenge as they involve both degrees of freedom. Although various approaches exist, comprehensive benchmarks comparing different methods and basis sets are still rare. In our study, we investigate two different methods to calculate the electron-phonon couplings. The first approach was developed by Engel et al. [1] and is based on the projector-argumented-wave formulation and maximally localized Wannier functions and is implemented in the VASP code. The second approach is based on a real-space description in terms of Gaussian basis functions and is implemented using cp2k. Both approaches use a finite-displacement and finite-difference scheme to calculate the coupling constants. We compare both methods using different molecules and discuss critical points for accurate calculations.

[1] Physical Review B 106, 094316 (2022)

HL 16.3 Tue 10:00 H14

Excitons in organic donor-acceptor cocrystals — •Sebastian Anhäuser[1], Ana Maria Valencia[2], Caterina Cocchi[2], and Gregor Witte[1] — [1]Philipps-Universität Marburg, FB Physik — [2]Carl von Ossietzky Universität Oldenburg, Institut für Physik

Organic donor-acceptor heterostructures have gained significant attention due to their unique properties, such as low-bandgap semiconductivity and ambipolar transport, making them promising candidates for optoelectronic applications like organic photovoltaics. There, the formation of charge-transfer excitons is typically regarded as the precursor state for charge separation. However, the microscopic nature of these excitons is not yet well understood. In the presented study, we perform detailed polarization-resolved optical spectroscopy on high quality acene-perfluoroacene donor-acceptor single crystals in the optical and UV range. This approach allows us to investigate both the excitation energies and the transition dipole moments of various (charge-transfer-)excitons. Using complementary state-of-the-art first principles calculations based on density functional and many-body pertubation theory, we analyse the nature of different classes of excitons within the cocrystalline structure. Our findings provide a refined understanding of charge-transfer excitons in organic materials, paving the way for improved design strategies in organic optoelectronics.

HL 16.4 Tue 10:15 H14

Detecting charge patterns on a novel type of rubrene crystals by time-of-flight photoemission electron microscopy — •Moha Naeimi[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]University of Rostock, Institute of physics, Rostock, Germany — [2]University of Rostock, Department of life, light and matter, Rostock, Germany

Organic molecules are increasingly drawing attention due to their broad applications, not only in organic field effect transistors and organic light emitting diodes [1], but also with respect to the exciton dynamics and charge transfer [2]. To this end, single crystalline domains with compact and stable molecular packing are beneficial. In this work, we focus on charge patterns and its dynamics for a recently discovered type of rubrene single crystals consisting of two distinct types of domains [3]. We show that both domains exhibit different charging properties, and that one of them can be controlled by photon exposure. This charge pattern can be *reset* by a second light source with lower photon energy, essentially neutralizing the charged sections. We tentatively attribute the behavior to the selective photo-injection of mobile excitons, resulting in spatially dependent conductivities.

[1] Wei-Cheng Su et al., Influence of Singlet and Charge-Transfer Excitons on the Open-Circuit Voltage of Rubrene/Fullerene Organic Photovoltaic Device ACS Appl. Mater. Interfaces, 8, 28757-28762 (2016) [2] Drew M. Finton et al., Routes to singlet exciton fission in rubrene crystals and amorphous films AIP Advances 9, 095027 (2019) [3] Moha Naeimi et al., Characteristics of zone-sectored tabular orthorhombic rubrene microcrystals in preparation.

HL 16.5 Tue 10:30 H14

Toward High Efficiency and Stable Blue OLEDs/Organic Light-Emitting Diodes with Lanthanide-Based Complexes: Host Material Impact — •Mahmoud Soleimani[1,2], Paulius Imbrasas[2], Sebastian Schellhammer[1], Carsten Rothe[2], and Sebastian Reineke[1] — [1]Institute for Applied Physics (IAP), Technische Universität Dresden, Germany — [2]beeOLED GmbH, Dresden, Germany

Lanthanides offer a new approach for achieving blue emission in organic light-emitting diodes (OLEDs). Cerium (III) and Europium (II) complexes emit in the blue range via the 5d-4f transition, potentially enhancing the stability and efficiency of OLEDs, outperforming current emitters. However, precise ligand design around the lanthanide is required for a stable, blue-emissive complex. With the right ligands, emitters with near-unity photoluminescence quantum yield in solution have been demonstrated. In the transition to OLED-compatible thin-films, we found that the host material plays a key role in maintaining this luminescence efficiency and that it can also impair emission through quenching mechanisms caused by unfavorable energy level alignment and coordination of the metal-organic complex by the host. This study investigates the photoluminescence of Cerium (III) tris(pyrazolyl)borate complex blended with four common OLED emission layer hosts. These insights guide the development of efficient blue OLEDs with lanthanide complexes.

HL 16.6 Tue 10:45 H14

Modifying the density of states in dipolar organic semiconductors — •Andrei Stankevich[1], Prakhar Sahay[3], Heinz Bässler[1], Wolfgang Brütting[3], Fabian Eller[2], Eva M.

Herzig[2], Andrey Kadashchuk[1], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth — [3]Institute of Physics, University of Augsburg,

Charge transport properties of amorphous organic semiconductors are controlled by energetic disorder. Certain device properties, such as the energies of charge transfer states in organic light-emitting diodes, can be improved by using dipolar molecules as host. Such molecules, however, also introduce interactions between charge carriers and randomly aligned dipoles. A key consequence of this is that increases the energetic disorder, hence causing a broad distribution of localized states, which hinders charge transport. We combined thermally stimulated luminescence studies with grazing incidence wide angle X-ray scattering, to demonstrate how the density of states in dipolar materials can be tailored. We demonstrate that the DOS is highly sensitive to the deposition technique and, consequently, the resulting film morphology. Furthermore, we show that the energetic disorder is not only determined by the static dipole moment, but also by the polarizability of charged molecules. Through this insight we derive design rules for common OLED materials that exhibit a with high dipole moments while maintaining charge transport properties comparable to those of non-polar counterparts.

15 min. break

HL 16.7 Tue 11:15 H14

Electrical and Optical Processes in Blue TADF OLEDs Studied by Temperature-Dependent Spectroscopy — •Ahmed Mohamed, Felix Kübert, Klara-Maria Bögle, Tolga Durmus, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, German

This study explores the electrical and photophysical processes in Thermally-Activated Delayed Fluorescence (TADF) Organic Light-Emitting Diodes (OLEDs) using temperature-dependent spectroscopic techniques. Key aspects such as charge carrier transport, current loss mechanisms and recombination dynamics are examined to provide a comprehensive understanding of device performance. We analyze current density-voltage-luminance (JVL) with respect to leakage current, efficiency roll-off, and current density at 90% external quantum efficiency *90. Electroluminescence (EL)/photoluminescence (PL) microscopy is employed to analyze the photophysical processes in OLEDs. EL spectra of blue OLEDs with the multi-resonance emitter *-DABNA exhibit remarkable spectral stability at temperatures between 200-300 K. Analysis of transient EL with rate equations yields activation energy and the rates of triplet-singlet transitions in OLEDs, including reverse intersystem crossing (rISC), triplet-triplet annihilation (TTA), and triplet-polaron annihilation (TPA). Understanding the mechanisms of current loss and (non-)radiative transitions is the prerequisite for enhancing the efficiency and stability of blue OLEDs.

HL 16.8 Tue 11:30 H14

Low Invasive Deposition of Metal Films on Carbon Nanotubes — •Martin Ernst[1,2], Martin Hartmann[1,2,3], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nano Technologies, Chemnitz University of Technology, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

Carbon nanotubes (CNTs) are one of the most promising materials for the next generation of electronics. Their unique one-dimensional electronic structure and their remarkable optical, thermal and mechanical properties makes them ideal candidates for different application scenarios. These range from the integration in transistors for analog and digital applications, as well as their usage in CNT-based gas, bio and stress sensors. One of the key challenges is the realization of a proper CNT-metal contact, in order to effectively transport charge carriers trough an electronic device, such as the carbon nanotube field-effect transistor (CNTFET). In this study we investigated the effects of different deposition parameters on the amount of lattice defects in single-walled semiconducting CNTs by Raman spectroscopy. There, a clear dependency between the amount of introduced defects and the deposition parameters, like the kinetic energy of the incident target atoms, was observed. Moreover, these finding were correlated to electrical results of CNTFETs, that were fabricated with the same deposition parameters.

HL 16.9 Tue 11:45 H14

High-Frequency CNT-based FETs for Radio Frequency Communication — •Martin Hartmann[1,2,3], Simon Böttger[1,2,3], Martin Ernst[1,2], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nanotechnologies, Chemnitz University of Technology, Germany — [2]Center for Materials Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nanosystems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

High frequency carbon nanotube-based (CNT) field effect transistors (FETs) are a highly promising candidate for future communication electronics due to their high charge carrier mobility and low intrinsic capacitance. It has already been shown in 2019 that this technology surpassed comparable silicon-based radio frequency FETs e.g. in terms of their extrinsic current gain cut-off frequencies as well as maximum frequencies of oscillation [1]. Moreover, in recent years their performance was further enhanced approaching the THz region [2]. We report on the impact of the device geometry as well as the CNT layer properties of high frequency CNTFETs onto their operating speed, linearity and contact resistance. Therefore, the spacers between the gate and the source electrode and gate to drain electrode were varied resulting in extrinsic current gain cut-off frequencies up to 14 GHz. By manipulating the spacer region, the device electrostatics in the CNT-metal contact area are balanced. This impacts the charge carrier injection and reflection at the Schottky-like barriers.

HL 17: 2D Semiconductors and van der Waals Heterostructures III

The session covers electronic and optoelectronic phenomena in two-dimensional semiconductors and van der Waals heterostructures.

Time: Tuesday 9:30–13:00 Location: H15

HL 17.1 Tue 9:30 H15

Size-Dependent Electrical Transport in Quasi-1D $ZrSe_3$-Stripes — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hannover, Germany

The anisotropy in form of quasi one-dimensional (1D) chains in transition metal trichalcogenides (TMTCs) makes them stand out compared to other more conventional two-dimensional (2D) materials [1]. Building on previous work [2], we investigated the electrical properties of thin stripes of the TMTC $ZrSe_3$ particularly regarding their width and thickness. The bulk material used was fabricated by a chemical vapor transport method and then exfoliated to achieve thin stripes.

We determined band gap energies for samples with varying heights. Those are shown to increase linearly from 0.37 eV to 0.63 eV as the thickness of the material decreases from 35 nm to 14 nm. Furthermore, we compared narrow samples with wider samples where both have comparably similar length and thickness and found that the conductivity happens dominantly in the outer selenium atoms i.e. across the chains.

[1] J. O. Island et al., 2D Materials 4, 0220033 (2017)
[2] L. Thole et al., ACS Omega 7, 39913-39916 (2022)

HL 17.2 Tue 9:45 H15

MOCVD Growth of two-dimensional, high-mobility InSe — •Robin Günkel[1], Milan Solanki[1], Daniel Anders[2], Markus Stein[2], Badrosadat Ojaghi Dogahe[1], Oliver Massmeyer[1], Max Bergmann[1], Nils Langlotz[1], Jürgen Belz[1], Sangam Chatterjee[2], and Kerstin Volz[1] — [1]Department of Physics and Material Sciences Center, Philipps-University Marburg, Germany — [2]Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus-Liebig-University Giessen, Germany

To advance Moore's Law, transistors must shrink while maintaining performance, but 3D semiconductor-based gates face limitations as their thickness approaches the nanometer scale due to surface scattering effects. 2D materials, such as graphene, offer a promising alternative that combines miniaturization with high field effect mobility. Among these, layered indium selenide (InSe) is a focus for logic devices due to its high mobility. However, the complex phase diagram of InSe poses challenges, often resulting in undesired phases. This study uses metal-organic chemical vapor deposition (MOCVD) to grow homogeneous, single-phase InSe on 2" sapphire by tuning the precursor ratio of DiPSe and TMIn. Growth starts with small nuclei forming a continuous layer, with subsequent layers growing as InSe triangles. Atomic force microscopy, Raman spectroscopy, STEM, and XRD provide insight into the growth behavior and the role of surface chemistry. Terahertz spectroscopy confirms carrier mobilities in the order of 1000 cm^2/(Vs). Ongoing efforts focus on heterostructures with other van der Waals materials to further tailor properties.

HL 17.3 Tue 10:00 H15

Transparent and reproducible contacts to MoS_2 nanotube quantum dots — •Robin T. K. Schock[1], Stefan B. Obloh[1], Korbinian Fink[1], Matthias Kronseder[1], Matjaž Malok[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Jožef Stefan Institute, 1000 Ljubljana, Slovenia

MoS_2, a leading material among transition metal dichalcogenides, exhibits remarkable optical and electronic properties. However, its high effective electron mass necessitates narrow confinement potentials to achieve single quantum level transport.

Nanotubes offer a compelling solution by naturally confining electrons in two dimensions. Our previous work demonstrated single level transport in nanotube QDs confined to the active device area, using the classical Scotch tape method.[1] Despite this, a major challenge remains in fabricating reliable electrical contacts, as devices still exhibit large resistance variations. We attribute this to the curved geometry of the nanotube surface, leading e.g. to nanogaps between the contact material on the tube and the chip surface.[2]

Here we introduce a contact deposition technique that addresses these challenges, achieving highly improved contact yield and reproducibility. This advancement enables the fabrication of more complex device architectures, as e.g., nanotube QDs on top of 2D material heterostacks. - [1] R. T. K. Schock et al., Adv. Mat. 35, 2209333 (2023); [2] R. T. K. Schock et al., PSSb, 2400366 (2024)

HL 17.4 Tue 10:15 H15

Defect engineering in two-dimensional materials for resistive switching — •Manoj Dey, Matthias Scheffler, and Wahib Aggoune — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft, Berlin, Germany

Non-volatile resistive switching (RS) in memristors has attracted significant attention for advancing in-memory technologies. Recently, exceptional RS has been observed in defected two-dimensional (2D) materials, called atomristors. Adsorption/desorption of metal atoms from the electrodes onto vacancy sites is experimentally observed and proposed as its origin [1,2]. Here, we explore the characteristics of defects and demonstrate their relationship with the observed RS. Using hybrid density functional theory with many body van der Waals corrections, we reveal that the defective monolayers are semiconducting (*i.e.*, high resistivity), whereas adsorption of metal atoms leads to a metallic character (*i.e.*, low resistivity). Interestingly, the adsorption energy of metal is found to be exothermic, with magnitude varying depending on the host materials. This indicates the feasible adsorption and switching in experiments. To bridge with experiments we also consider both the effects of the electrode (*e.g.* Au(111)) and finite-temperature vibrations. While vibrational effects are negligible, electrode screening induces band gap renormalization and slightly stabilizes metal adsorption compared to free-standing monolayers. These insights will guide the exploration of novel 2D materials for RS applications.

[1] Ruijing Ge *et al.*, *Adv. Mater.*, **33**, 2007792 (2021).
[2] Saban M. Hus *et al.*, *Nat. Nanotechnol.*, **16**, 58 (2021).

HL 17.5 Tue 10:30 H15

Anisotropic supercurrent suppression and revivals in a graphene-based Josephson junction under in-plane magnetic fields — •Katarina Stanojević[1,5], Philipp Schmidt[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Bernd Beschoten[1], Vincent Mourik[5], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Research Center for Electronic and Optical Materials, National Institute for Materials Science, Japan — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan — [5]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany

Graphene-based Josephson junctions represent a promising platform for hybrid quantum devices due to their unique electronic properties. The absence of Schottky barriers enables highly transparent interfaces, while graphene's ability to host proximity-induced superconductivity make it an interesting candidate for realizing tunable weak links. A key step towards harnessing graphene Josephson junctions for topological quantum applications is understanding the influence of in-plane magnetic fields, which tune the Zeeman energy and might enable the formation of topologically protected states. Here, we report on a tunable bilayer graphene Josephson junction encapsulated in WSe_2. We investigate the behavior of the supercurrent under applied in-plane magnetic fields, revealing a pronounced anisotropy in the magnetic field induced decay and revival of the supercurrent for varying in-plane field angles.

HL 17.6 Tue 10:45 H15

Electric field control of the proximity-induced spin-orbit gap in bilayer graphene/WSe2 quantum dots — •Hubert Dulisch[1,2], David Emmerich[1,2], Eike Icking[1,2], Katrin Hecker[1,2], Samuel Möller[1,2], Leonie Müller[1,2], Kenji

Watanabe[3], Takashi Taniguchi[4], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]2nd Institute of Physics, RWTH Aachen — [2]PGI-9, Forschungszentrum Jülich — [3]Research Center for Functional Materials, NIMS, — [4]International Center for Materials Nanoarchitectonics, NIMS

We investigated induced spin-orbit coupling (SOC) in a bilayer graphene (BLG) quantum dot (QD), which is in proximity to tungsten diselenide (WSe_2). Magneto-transport measurements were performed on the Coulomb-resonance of the first charge carrier to extract the spin-orbit gap Δ_{SO}. In-plane magnetic field measurements indicate an increased SOC-induced energy splitting. Out-of-plane field measurements demonstrate a reduced valley g-factor at larger displacement fields, consistent with weaker lateral confinement of the QD wavefunction. Our measurements reveal an enhanced SOC effect that decreases with the applied displacement field, distinguishing it from the behavior observed in pure BLG. We interpret this as a reduced influence of the WSe_2, which we attribute to the increased displacement field. This causes the QD to become more localized in the lower layer of the bilayer graphene. Being farther from the WSe_2, this layer experiences reduced induced SOC, leading to a diminished spin-orbit gap in the BLG QD.

HL 17.7 Tue 11:00 H15

High-Performance and Energy-Efficient Sub-5nm 2D Double-Gate MOSFETs Based on SiAs Monolayers — •Dogukan Hazar Ozbey and Engin Durgun — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey

As the demand for high-performance, energy-efficient transistors grows, traditional silicon-based MOSFETs face significant scaling limitations. To overcome these challenges and sustain advancements in semiconductor technology, new materials and device architectures are being explored. In this study, sub-5nm double-gate metal-oxide-semiconductor field-effect transistors (MOSFETs) based on 2D SiAs are investigated using first-principles calculations and the Non-equilibrium Green's function (NEGF) formalism to assess their potential as a high-performance alternative. SiAs monolayers exhibit an indirect bandgap of 1.58 eV and demonstrate promising electronic properties. Key performance metrics such as the on/off current ratio, subthreshold swing (SS), gate capacitance (C_g), intrinsic delay time (τ), and power-delay product (PDP) are evaluated. Devices with 1 nm and 2 nm underlap (UL) structures show enhanced performance, achieving on-state current (I_{on}) values up to 1206 $\mu A/\mu m^{-1}$, meeting ITRS-2028 high-performance (HP) standards. The SS ranges from 112 to 142 mV/dec, and minimized delay and power-delay products indicate the suitability of SiAs transistors for ultra-scaled, energy-efficient applications. Results suggest that 2D SiAs transistors offer a promising solution to the scaling challenges of MOSFET technologies.

15 min. break

HL 17.8 Tue 11:30 H15

Resistance standards from artifact wire coils to graphene quantum Hall resistance — •Yefei Yin[1], Mattias Kruskopf[1], Stephan Bauer[1], Teresa Tschirner[1], Klaus Pierz[1], Frank Hohls[1], Rolf J. Haug[2], and Hans W. Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Historically, resistance standards were made by physical artifact wire coils before 1990 and quantum resistors based on GaAs heterostructures after 1990. However, conventional GaAs quantum Hall resistance (QHR) standards with the quantized resistance $R_H = h/2e^2$ are operating under high magnetic flux densities B > 10 T, limited currents I < 50 μA, and low temperatures T < 1.5 K, which significantly hinder the dissemination of primary resistance standards. In this work, we developed practical primary QHR standards based on n- and p-type epitaxial graphene. This study first systematically demonstrated that p-type epitaxial graphene can also be used for primary resistance standards, as accurate (10^{-9} accuracy) as GaAs and n-type graphene counterparts for realizing the SI unit ohm in quantum metrology. [1] The n-type graphene QHR standards achieved the world best performance so far with a 10^{-9} accuracy under relaxed conditions (B = 4.5 T, I = 232.5 μA, T = 4.2 K) simultaneously. [2-3] Our graphene QHR standards have been utilized in the national metrology institutes in European countries. [1] Appl. Phys. Lett., 125, 064001 (2024). [2] Adv. Phys. Res. 1, 2200015 (2022). [3] Phys. Rev. Applied, 2024

HL 17.9 Tue 11:45 H15

1D graphene superlattices and the influence of the potential shape — •Julia Amann[1], Alina Mreńca-Kolasińska[2], Angelika Knothe[1], Ming-Hao Liu[3], Takashi Taniguchi[4], Kenji Watanabe[4], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Germany — [2]AGH University, Krakow, Poland — [3]National Cheng Kung University, Tainan, Taiwan — [4]National Institute for Materials Science, Tsukuba, Japan

One-dimensional superlattices (1DSLs) in graphene have been predicted to exhibit intriguing effects such as transport anisotropy, additional Dirac points and hence higher degeneracy, leading to a different quantum Hall plateau sequence compared to pristine graphene. We use a patterned few-layer graphene gate under an encapsulated monolayer graphene to fabricate a 1DSL device. With the combined effect of a global gate and a patterned bottom gate, we are able to control the superlattice potential strength and carrier density independently. We show low-temperature transport measurements on a gate-tunable 1DSL in monolayer graphene with a period of 50 nm in directions parallel and perpendicular to the modulation using an L-shaped Hall bar. We observe anisotropic transport and the appearance of multiple Dirac points and additional Landau fans in the modulation direction. We also see Weiss oscillations, confirming the 1DSL modulation. However, the predicted anomalous quantum Hall sequence was not observed and we looked more closely at the 1DSL potential we were applying. We found an asymmetric potential shape, which strongly influences the change in the band structure and degeneracy.

HL 17.10 Tue 12:00 H15

Ultrafast mid-infrared interferometric photocurrents in graphene-based two-terminal devices for femtosecond autocorrelation — •Sebastian Loy[1,2], Nina Pettinger[1,2], Johannes Schmuck[1,2], Xiaoyi Zhou[1,2], Sergey Zherebtsov[1,2], Christoph Kastl[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center of Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

We present the autocorrelation of femtosecond mid-IR pulses with wavelengths ranging from 5.5 μm to 14 μm and pulse durations of approximately 100 fs on graphene-based two-terminal devices. The results indicate that the interaction between the electric field and optoelectronic dynamics at the metal-graphene interface underlies the principle of ultrafast detection. Our approach stands out due to the ease of nanofabricating graphene two-terminal optoelectronic devices and their inherent robustness [1].

[1] Nina Pettinger et al., accepted (2024).

HL 17.11 Tue 12:15 H15

Enhancement of optoelectronic properties of layered 2D semiconductors — •Borna Radatović[1,2], Onur Çakiroğlu[2], Hao Li[2], Fedor Lipilin[1], Aljoscha Soll[1], Andres Castellanos-Gomez[2], and Zdenek Sofer[1] — [1]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, Prague 6, 166 28 Czech Republic — [2]2D Foundry group. Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), E-28049 Madrid, Spain

Standard semiconductor methods for the enhancement of electronic devices' properties, such as doping via ion implantation and similar approaches, do not apply to 2D materials due to their atomical thickness. However, various alternative methods for customization of optoelectronic properties of 2D devices have been investigated, from electric or magnetic fields to substitutional doping, that were demonstrated for many devices, such as light sources, optical modulators and photodetectors. In our work, we focus on photodetectors based on different 2D semiconductors (i.e. MoS2, ZrSe3, Sb2S2O and CuInP2Se6) in monolayer and few-layer forms. We investigated how external strain can modulate the intrinsic optical and electronic properties of 2D materials and enhance photodetectors' performances. Furthermore, we have demonstrated how 2D heterostructures can offer a practical approach to specific custom optoelectronic properties of 2D devices.

HL 17.12 Tue 12:30 H15

Surface acoustic wave-controlled photocurrent in few-layer TMDCs — •Benjamin Mayer, Felix Ehring, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten —

Institute of Physics, University of Münster, Germany

Surface acoustic waves (SAWs) provide a versatile platform for integrating GHz-frequency control and sensing schemes at micron-scale wavelengths on a chip. Combining the SAWs dynamic electric field, high-resolution optical spectroscopy, and electrical transport allows a deep insight in the optical properties and carrier transport processes in nanoscale materials, paving the way for innovative acousto-optoelectronic devices [1].

Here, we study the SAW-driven acousto-electric current (AEC) and the underlying charge carrier dynamics in mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials. To this aim, few-layered TMDCs are placed on top of two gold electrodes integrated in hybrid lithium niobate-based SAW-devices with design frequencies of 150-250MHz. The power and directional dependence of the induced AEC offer an initial understanding of the contact barriers forming at the Au-TMDC interface. By locally photodoping our samples, we establish a qualitative model for the formed Schottky and tunneling barriers, enabling the investigation of their influence on the wavelength-dependent SAW-driven charge carrier dynamics [2].

[1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)
[2] Adv. Mater. 2402799 (2024)

HL 17.13 Tue 12:45 H15

Accelerated electron-hole separation at the organic-inorganic anthracene/Janus MoSSe interface — •Hamid Mehdipour[1], Peter Kratzer[2], and Oleg Prezhdo[3] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]University of Duisburg-Essen, Duisburg, Germany — [3]University of Southern California, Los Angeles, United States;

Organic light-absorbing materials with two-dimensional semiconductor layers as contact electrodes are promising for efficient and low-cost energy-harvesting applications. Considering anthracene as an absorber and a MoSSe Janus monolayer, and basing our work on a set of preliminary DFT calculations, we employ non-adiabatic molecular dynamics to show that electron transfer from anthracene to MoSSe is faster on the Se than on the S side. The transfer from anthracene to MoS_2 and $MoSe_2$ monolayers takes intermediate times. As a rule, we find that a shorter adsorption distance produces a stronger donor-acceptor coupling. The smaller distance on the Se side is rationalized by the attractive dipolar interaction between the intrinsic dipole moment of the Janus structure and the dipole induced upon molecule adsorption. Quantum coherence adjusted by the out-of-plane vibrations also has a significant impact on the transfer time. Our study provides detailed insights into adsorption of molecules on Janus structures and the resulting electronic and electron-vibrational interactions. The results suggest that the dipole interaction plays an important role in thermodynamic stability, alignment of electronic levels, and electron-vibrational dynamics.

HL 18: Focus Session: Nanoscale Light-matter Interaction I

The focus session highlights recent breakthroughs in resolving the optoelectronic properties of individual nanostructures down to the atomic scale. Moreover, the session introduces the rich field of surface polaritons, confined electromagnetic modes through which light can be guided on subwavelength scales.

The focus session is organized by Markus Huber (U Regensburg) and Fabian Mooshammer (U. Regensburg).

Time: Tuesday 9:30–13:00 Location: H17

Invited Talk HL 18.1 Tue 9:30 H17

Ultrafast Nano-Spectroscopy of Photo-Induced Dynamics in Low-Dimensional Materials — •Takashi Kumagai — Institute for Molecular Science, Okazaki, Japan

Low-dimensional semiconductors have been extensively studied as platforms for fascinating physics and as potential components for quantum nano-devices. Their low dimensionality leads to unique physical properties, driven by strong quantum confinement and reduced dielectric screening. However, this also renders low-dimensional materials highly sensitive to local structures and interactions with their surroundings. To fully understand their superior properties, it is essential to investigate their local structures and how they correlate with photo-induced dynamics. Recently, ultrafast infrared nano-spectroscopy based on scanning near-field optical microscopy (IR-SNOM) has emerged as a powerful tool to directly visualize local structures and dynamics in real time and space at the nanoscale. I will present our latest research to apply ultrafast IR-SNOM to explore nanoscale photo-induced dynamics in low-dimensional materials [1]. In single-layer transition metal dichalcogenides, we have visualized the local many-body dynamics of high-density electron-hole plasma, uncovering the significance of dynamic heterogeneity linked to the non-uniform optoelectronic properties. Furthermore, we have extended ultrafast IR-SNOM to study local exciton dynamics in single-walled carbon nanotubes (SWCNTs). Within individual, isolated SWCNTs, the non-uniform formation of electron-hole pairs is correlated with local strain. [1] Y. Wang, J. Nishida et al. ACS Photonics, accepted.

Invited Talk HL 18.2 Tue 10:00 H17

Landau level Nanoscopy of charge and heat transport in low-dimensional heterostructures — •Mengkun Liu — Stony Brook University

In contemporary condensed matter physics and photonics, four key length scales play an essential role in shaping the behavior of quantum materials: (1) the polaritonic wavelength, which governs light confinement and light-matter interactions; 2) the magnetic lengths, determined by the magnetic field B, which constrains electron motion; 3) the diffusion length of the hot carriers at interfaces and the edges, which dictates energy relaxation, and 4) the periodicities of superlattices induced by moiré engineering, which defines the energy scale of emerging quantum phases. For instance, the commensurability of the magnetic lengths (~10 nm for graphene at 7T) and superlattice constant (~10 nm for twisted bilayer graphene at "magic" angle) would give rise to exotic fractal quantum states. In this talk, I will present: 1) A cutting-edge optical spectroscopy technique, Landau-level nanoscopy, capable of simultaneously probing all four critical length scales in a single experiment; 2) the discovery of classes of infrared polaritons that can be tuned by magnetic fields, enhancing our ability to manipulate light-matter interactions and probe many-body physics at the nanoscale; 3) nanoscale mapping of thermoelectric properties in the quantum Hall bulk, revealing strong violations of the Wiedemann-Franz law. Our approach establishes Landau-level nanoscopy as a versatile platform for investigating magneto-optical effects and many-body interactions at the nanoscale.

Invited Talk HL 18.3 Tue 10:30 H17

Real space mapping of electrically tunable anisotropic THz plasmon polaritons in hBN encapsulated black phosphorus — •Eva Pogna — Institute of Photonics and Nanotechnology, CNR-IFN, Milan, Italy

Polaritons in two-dimensional layered crystals offer effective means to confine and manipulate terahertz (THz) electromagnetic waves at the nanoscale, a crucial step in advancing photonic technologies.

In this study, we investigate anisotropic plasmon polaritons in black phosphorus nanoflakes at THz frequencies, utilizing near-field photocurrent nanoscopy combined with THz hyperspectral near-field scattering techniques.

Encapsulation with hexagonal boron nitride protects black phosphorus from air-induced degradation, while field-effect transistor (FET) devices enable photo-thermoelectric detection of plasmon polaritons.

Our findings reveal highly confined, gate-tunable plasmon polaritons with subwavelength dispersion ($\sim \lambda/76$ at 2.01 THz).

The dielectric anisotropy of black phosphorus leads to polaritons with elliptic wavefronts at THz frequencies, enabling enhanced confinement and control over THz field propagation. Moreover, electrostatic control of carrier density allows precise tuning of polariton wavelength, highlighting the versatility of this platform for nanoscale THz light ma-

nipulation and reconfigurable infrared nanophotonics.

Notably, the four-gate FET architecture introduced here to examine in-plane propagation anisotropy can be readily adapted for the study of other anisotropic conductive materials.

15 min. break

Invited Talk HL 18.4 Tue 11:15 H17

Ultra-confined THz hyperbolic phonon polaritons in a transition metal dichalcogenide — Ryan A. Kowalski[1], Niclas S. Mueller[2], Gonzalo Alvarez-Perez[3], Maximilian Obst[4], Katja D. Granados[1], Giulia Carini[2], Aditha Senarath[1], Saurabh Dixit[1], Richarda Niemann[1,2], Ragu B. Iyer[5], Felix Kaps[4], Jakob Wetzel[4], J. Michael Klopf[6], Ivan I. Kravchenko[7], Deliang Bao[1], Sokrates T. Pantelides[1], Martin Wolf[2], Lukas Eng[4], Pablo Alonso-Gonzalez[3], Susanne Kehr[4], Thomas G. Folland[5], •Alexander Paarmann[2], and Joshua D. Caldwell[1] — [1]Vanderbilt University, Nashville, TS, USA — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [3]University of Oviedo, Oviedo, Spain — [4]TUD Dresden University of Technology, Dresden, Germany — [5]The University of Iowa, Iowa City, IA, USA — [6]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [7]Oak Ridge National Laboratory, TN, USA

Phonon polaritons are hybrid light-matter quasiparticles in polar crystals that enable waveguiding of light on length scales much smaller than the photon wavelength. Here, we introduce $HfSe_2$ as a new van der Waals material that supports phonon polaritons in the terahertz (THz) spectral range. Using THz near-field optical microscopy, we demonstrate extreme confinement of light from 61 μm free-space wavelength to 245 nm. We show that the origin of this record-high confinement is an exceptionally large light-matter coupling of hyperbolic $HfSe_2$.

Invited Talk HL 18.5 Tue 11:45 H17

Programmable polariton nanophotonics using phase-change materials — •Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

Tailoring light-matter interaction is essential to realize nanophotonic components and can be achieved with polaritons, an excitation of photons coupled to charges in metals and semiconductors. Adding a thin layer of Phase-change material (PCM) leads to stronger polariton confinement and enables optical writing of resonator structures based on a change in the refractive index [1]. The recently introduced plasmonic PCM In_3SbTe_2 (IST) can be reversibly switched from an amorphous dielectric to a crystalline metallic state, enabling optically re-writable IR nanoantennas and metasurfaces [2].

Here, we show direct optical writing of resonators for surface phonon polariton (SPhP) by crystallizing IST on top of a SiC crystal and investigate the strongly confined resonance modes with s-SNOM. Reconfiguring the size and shape of the resonators leads to mode confinements of $\lambda/35$ [3]. We also demonstrate the real-space imaging of IR surface plasmon polaritons on bulk doped semiconductors, enabled by the strong polariton confinement induced by the added thin dielectric PCM layer [4]. Our concept allows for the rapid prototyping of reconfigurable structures for polaritonics, especially useful with anisotropic 2d materials.

[1] Li et al., *Nat. Mat.* **15**, 870 (2016) [2] Heßler et al. *Nat. Com.* **12**, 924 (2021) [3] Conrads et al. *Nat. Com.* **15**, 3472 (2024) [4] Conrads et al. *Sci. Adv. under review*

HL 18.6 Tue 12:15 H17

Heralding non-classical light by tailored free-electron interactions with photonic modes — •Armin Feist[1,2], Guanhao Huang[3,4], Germaine Arend[1,2], Yujia Yang[3,4], Jan-Wilke Henke[1,2], Zheru Qiu[3,4], Hao Jeng[1,2], Arslan Sajid Raja[3,4], Rudolf Haindl[1,2], Rui Ning Wang[3,4], Tobias J. Kippenberg[3,4], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, DE — [2]4th Physical Institute, University of Göttingen, DE — [3]Institute of Physics, EPFL, Lausanne, CH — [4]Center for Quantum Science and Engineering, EPFL, Lausanne, CH

Integrated photonics facilitates control over fundamental light-matter interactions in manifold quantum systems. Extending these capabilities to electron beams [1] fosters free-electron quantum optics.

Here, we show the coupling of single electrons and photons at an integrated photonics waveguide [2,3]. Spontaneous scattering of the nanoscale-focused electron beam at empty optical modes creates multi-photon superposition states. Energy-selective and event-based electron detection enables heralding non-classical light, which we characterize by intensity correlations in a Hanbury Brown and Twiss (HBT) setup, showing high-fidelity single-photon generation [3].

This provides a pathway toward novel hybrid quantum technology with entangled electrons and photons, as well as the capability for quantum-enhanced electron imaging and Fock-state photon sources.

[1] J.-W. Henke *et al.*, Nature **600**, 653 (2021). [2] A. Feist *et al.*, Science **377**, 777 (2022). [3] G. Arend *et al.*, arXiv:2409.11300 (2024)

HL 18.7 Tue 12:30 H17

Attosecond electron microscopy using free-electron homodyne detection — •John H. Gaida[1,2], Sergey V. Yalunin[1,2], Hugo Lourenço-Martins[1,2], Murat Sivis[1,2], Thomas Rittmann[1,2], Armin Feist[1,2], F. Javier García de Abajo[3,4], and Claus Ropers[1,2] — [1]MPI for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany — [3]ICFO-Institut de Ciencies Fotoniques, Castelldefels (Barcelona), Spain — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

Advancements in condensed matter science aim to map material structures and dynamics at levels of ångströms and attoseconds. Although X-ray and electron methods offer structural detail, attosecond temporal resolution is progressing through optical spectroscopy techniques. Techniques like PINEM allow nanometric resolution imaging of near-field intensities [1], but to examine the evolution of nanoscale fields and structures within the light cycle, optical phase sensitivity is needed, as provided by phase-contrast Lorentz PINEM [2], interferometric detection [3], or electron pulse bunching [4]. This contribution introduces Free-Electron Homodyne Detection (FREHD), a universally applicable approach for high spatiotemporal resolution imaging of phase-resolved optical responses [3].

[1] B. Barwick *et al.*, Nature **462**, 902–906 (2009). [2] J. H. Gaida *et al.*, Nat. Commun. **14**, 6545 (2023). [3] J. H. Gaida *et al.*, Nat. Photonics **18** 509–515 (2024). [4] K. E. Priebe *et al.*, Nat. Photon. **11**, 793–797 (2017).

HL 18.8 Tue 12:45 H17

Light-matter interaction on subcycle time and atomic length scales — •Tom Siday[1,2], Johannes Hayes[1], Felix Schiegl[1], Fabian Sandner[1], Peter Menden[1], Valentin Bergbauer[1], Martin Zizlsperger[1], Svenja Nerreter[1], Sonja Lingl[1], Jascha Repp[1], Jan Wilhelm[1], Markus A. Huber[1], Yaroslav A. Gerasimenko[1], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham, UK

Near-field microscopy has revolutionized the study of nanoscale light-matter interaction, achieving subcycle temporal and ~10 nm spatial resolution. However, the geometry of the tip apex has so far restricted access to atomic resolution. By harnessing extreme nonlinearities within tip-confined evanescent light fields, we introduce a novel contrast mechanism, advancing all-optical microscopy to the atomic scale while preserving subcycle temporal resolution. This Near-field Optical Tunnelling Emission (NOTE) microscope can resolve nanometer-scale packing defects on a gold surface and trace the subcycle quantum flow of electrons between the scanning tip and a semiconducting van der Waals trilayer in real time. Moreover, NOTE microscopy is compatible with insulating samples, where rectified currents cannot flow, and enables the integration of all-optical subcycle spectroscopy with atomic-scale resolution. Thus, NOTE provides direct access to atomic-scale quantum light-matter interactions and dynamics on their natural spatial and temporal scales.

HL 19: Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)

In recent years, significant progress has been made in realizing and exploring correlated quantum states in multilayer moiré heterostructures of graphene or transition metal dichalcogenides. These achievements have been made possible by the high level of control and tunability of these systems. Striking phenomena have been demonstrated experimentally, including unconventional superconductivity, fractional quantum anomalous Hall states, Mott-Wigner states and density waves, as well as kinetic ferromagnetism. Moreover, recently novel spectroscopic experimental techniques have been developed which allow for new ways to explore the dynamical response of these exotic states. This focus session will discuss recent experimental advancements as well as theoretical developments in the field of strongly correlated moiré heterostructures.

Organizers: Dmitri K. Efetov (LMU München), Michael Knap (TU München)

Time: Tuesday 9:30–13:15 Location: H36

Topical Talk HL 19.1 Tue 9:30 H36

The Thermoelectric Effect and Its Natural Heavy Fermion Explanation in Twisted Bilayer and Trilayer Graphene — Dumitru Calugaru[1], Haoyu Hu[2], Rafael Luque Merino[3], Nicolas Regnault[4], Frank Koppens[3], Dmitri K. Efetov[5], and •Bogdan Andrei Bernevig[1] — [1]Dept of Physics, Princeton University, Princeton, USA — [2]DIPC, San Sebastián, Spain — [3]ICFO, Barcelona, Spain — [4]Laboratoire de Physique de l'ENS, Paris, France — [5]LMU Munich, Munich, Germany

We study the interacting transport properties of twisted bilayer graphene (TBG) using the topological heavy-fermion (THF) model, where TBG comprises localized, correlated f-electrons and itinerant, dispersive c-electrons. The Seebeck coefficient of TBG exhibits unconventional traits: negative values with sawtooth oscillations at positive fillings, contrasting typical band-theory expectations. This behavior arises from the dichotomy between heavy (short-lived, correlated f-electrons) and light (long-lived, dispersive c-electrons), with transport dominated by c-electrons due to their stronger dispersion and longer lifetimes. At positive integer fillings, c- (f-)electron bands govern the electron (hole) doping side, resulting in an overall negative Seebeck coefficient. Sawtooth oscillations occur near each integer filling due to gap openings. Our results underscore the importance of electron correlations and lifetime asymmetry, naturally captured by the THF model, in understanding TBG transport properties. These findings align with experiments on twisted bilayer and trilayer graphene and highlight the interplay of heavy and light carriers.

Topical Talk HL 19.2 Tue 10:00 H36

Angle-Tuned Chiral Phase Transition in Twisted Bilayer Graphene — •Laura Classen[1,2], Nikolaos Parthenios[1,2], Cheng Huang[3], Xu Zhang[3], Maksim Ulybyshev[4], Fakher Assaad[3], and Zi Yang Meng[4] — [1]Max Planck Institute for Solid State Research — [2]Technical University of Munich — [3]University of Hong Kong — [4]University of Wuerzburg

The twist angle constitutes an important control knob in twisted bilayer graphene that has become accessible in-situ. It effectively tunes between weakly interacting, decoupled graphene layers and strongly correlated electrons at a magic angle of around 1.1 degree. We propose that this facilitates the realisation of a chiral phase transition of Dirac fermions at charge neutrality in twisted bilayer graphene. We argue that the transition can be described by the Gross-Neveu-Yukawa model that couples Dirac fermions and an XY order parameter field. The quantum critical behavior of this effective model is consistent with quantum Monte Carlo simulations of the continuum model for twisted bilayer graphene.

Topical Talk HL 19.3 Tue 10:30 H36

Quantum Optics of Semiconductor Moire Materials — •Atac Imamoglu — Institute of Quantum Electronics, ETH Zurich

Moire superlattices in two dimensional semiconductors have enabled the observation of a wealth of phenomena driven by strong electronic correlations, ranging from Mott-Wigner states to fractional quantum anomalous Hall effect. In this talk, I will present experiments exploring quantum optical control of strongly correlated electrons.

15 min. break

Topical Talk HL 19.4 Tue 11:15 H36

Probing the Band Structures of Multilayer Graphene Using the Quantum Twisting Microscope — •Martin Lee[1,2], Ipsita Das[1,2], János Papp[1,2], Marc Currle[1], Jiazhuo Li[1,2], Mudit Bhatt[1,2], Jonah Herzog-Arbeitman[3], Jiabin Yu[3], Zhiyuan Zhou[3], Markus Becherer[4], Philipp Altpeter[1], Christian Obermayer[1], Heribert Lorenz[1], Kenji Watanabe[5], Takashi Taniguchi[5], Bogdan Andrei Bernevig[3,6,7], and Dmitri Efetov[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Department of Physics, Princeton University, Princeton, New Jersey, USA — [4]School of Computation Information and Technology, Technical University of Munich, Germany — [5]National Institute of Material Sciences, Tsukuba, Japan — [6]Donostia International Physics Center, Donostia-San Sebastian, Spain — [7]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Understanding the band-structure is foundational in describing the behavior of electrons in crystalline systems. While the tight-binding model effectively captures the non-interacting band-structures in materials like graphene, it relies on analytically or numerically derived hopping parameters. In this talk, we present the development of a quantum twisting microscope (QTM), which allows the k-resolved tunneling spectroscopy between the electronic states at the 2D tip and the 2D sample by twisting in-situ. Our QTM measurements allow us to extract the hopping parameters that agree with theoretical predictions.

Topical Talk HL 19.5 Tue 11:45 H36

Gate-Tunable Bose-Fermi Mixture in a Strongly Correlated Moiré Bilayer Electron System — •Nathan Wilson[1], Amine Ben Mhenni[1], Wilhelm Kadow[2], Mikołaj Metelski[1], Adrian Paulus[1], Alain Dijkstra[1], Jonathan Finley[1], and Michael Knap[2] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]School of Natural Sciences, TU Munich, Garching, Germany

Quantum gases consisting of species with distinct quantum statistics, such as Bose-Fermi mixtures, can behave in a fundamentally different way than their unmixed constituents. This makes them an essential platform for studying emergent quantum many-body phenomena such as mediated interactions and unconventional pairing. Here, we realize an equilibrium Bose-Fermi mixture in a bilayer electron system implemented in a WS_2/WSe_2 moiré heterobilayer with strong Coulomb coupling to a nearby moiré -free WSe2 monolayer. Absent the fermionic component, the underlying bosonic phase manifests as a dipolar excitonic insulator. By injecting excess charges, we show that the bosonic phase forms a stable mixture with added electrons but abruptly collapses upon hole doping. We develop a microscopic model to explain the unusual asymmetric stability with respect to electron/hole doping. By monitoring excitonic resonances from both layers, we demonstrate stability of the phase over a wide range in the boson/fermion density phase space, in agreement with theoretical calculations. Our results further the understanding of phases stabilized in moiré bilayer electron systems and demonstrate their potential for exploring the exotic properties of equilibrium Bose-Fermi mixtures.

HL 19.6 Tue 12:15 H36

Theory for Optical Control of Correlated States in

Moiré Transition Metal Dichalcogenide Heterostructures — •Haoyang Tian and Urban Friedrich Peter Seifert — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany

In recent years, moiré transition metal dichalcogenide (TMD) heterostructures have emerged as highly versatile platforms for investigating phases and phenomena of strongly correlated electrons on emergent lattice scales. However, experimental characterization of the precise nature of some interaction-driven long-range ordered states and their excitations has remained a challenge. Given strong light-matter couplings and valley selection rules in TMD materials, ultrafast optical methods may constitute a promising avenue for probing and controlling these states and their collective modes. In this work, we develop a theoretical framework to describe coherent light-matter interactions in moiré TMD heterostructures, and model the system's steady-state and non-equilibrium dynamics during and after photoexcitation with a laser pulse. Thus obtained characteristic signatures of the system's dynamics may allow for new experimental insights.

HL 19.7 Tue 12:30 H36

Single-Particle Spectral Function of Fractional Quantum Anomalous Hall States — •Fabian Pichler[1,2], Wilhelm Kadow[1,2], Clemens Kuhlenkamp[3,1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Department of Physics, Harvard University, Cambridge, Massachusetts, USA

Fractional quantum Hall states are the most prominent example of states with topological order, hosting excitations with fractionalized charge. Recent experiments in twisted $MoTe_2$ and graphene-based heterostructures provide evidence of fractional quantum anomalous Hall (FQAH) states, which spontaneously break time-reversal symmetry and persist even without an external magnetic field. Understanding the unique properties of these states requires the characterization of their low-energy excitations. To that end, we construct a parton theory for the energy and momentum-resolved single-particle spectral function of FQAH states. We explicitly consider several experimentally observed filling fractions as well as a composite Fermi liquid in the half-filled Chern band. The parton description captures qualitatively our numerical exact diagonalization results. Additionally, we discuss how the finite bandwidth of the Chern band and the non-ideal quantum geometry affect the fractionalized excitations. Our work demonstrates that the energy and momentum-resolved electronic single-particle spectral function provides a valuable tool to characterize fractionalized excitations of FQAH states in moiré lattices.

HL 19.8 Tue 12:45 H36

Tuneability of Superconducting Properties in Transition Metal Dichalcogenide bilayers — •Michael Winter and Tim O. Wehling — I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg

In recent years, rising interest sustained in van der Waals materials, particularly in transition metal dichalcogenides (TMDs or TMDCs). This work explores the potential for bilayer [hetero-]structuring in TMDs, which have garnered significant attention due to the discovery and prediction of exotic quantum phases, such as superconductivity and Mott insulating behaviour.

I present predictions derived from a minimal quantum lattice model, incorporating ab initio calculations based on plane-wave density functional theory (DFT), density functional perturbation theory (DFPT), and subsequent electron-phonon interaction calculations. The resulting model allows us to investigate the effects of different material combinations (e.g., MoS_2, $MoSe_2$, WS_2, WSe_2) and electron doping on superconductivity in such [hetero-]bilayer.

HL 19.9 Tue 13:00 H36

Proximity-Induced Spin-Triplet Superconducting Correlations in Transition Metal Dichalcogenides — •Florian Kayatz, Jorge Cayao, and Annica Black-Schaffer — Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

The realization of spin-triplet Cooper pairs is a key ingredient for superconducting spintronics. One promising route to achieve this task is by exploiting the strong intrinsic spin-orbit coupling of transition metal dichalcogenides (TMDs). In this work, we consider a TMD layer coupled to a conventional spin-singlet s-wave superconductor and demonstrate the emergence of spin-triplet superconducting correlations. We find that these spin-triplet pair correlations form in the TMD as a proximity-induced effect but also appear in the superconductor as an inverse proximity effect and as a nonlocal phenomenon that exists between the TMD and superconductor. Furthermore, we relate these emergent superconducting correlations to experimentally observable features in the density of states and conductance.

HL 20: Poster I

The first poster session covers the physics of semiconductor heterostructures, interfaces and surfaces. Moreover, most recent results on oxide semiconductors, as well as perovskite and photovoltaics are presented.

Time: Tuesday 10:00–12:30 Location: P3

HL 20.1 Tue 10:00 P3

Accuracy Requirements for Polarizabilities in MD-based Raman Spectra — •Markus Amaseder[1], Manuel Grumet[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Faculty of Natural Sciences, Comenius University Bratislava — [3]Institute of Inorganic Chemistry, Slovak Academy of Sciences

Raman spectroscopy provides a versatile and accessible method for characterizing atom dynamics in materials. While frozen phonon approaches have proven well for the prediction of Raman spectra in many cases, they do not inherently include anharmonic and temperature-dependent effects. Raman spectra calculated from molecular dynamics (MD) offer an alternative [1] and have received considerable interest. However, they remain computationally challenging as they require many single-point polarizabilities. We have shown previously that machine learning (ML) can aid in the speed-up using a delta learning approach [2]. However, it is still to be fully understood how accurate single-point polarizabilities need to be in order to provide sufficiently correct spectra. We present an evaluation of polarizabilities from density functional theory and ML for MD Raman spectra, investigating the effects of the functional and further parameters. This is relevant both in terms of training data and ML predictions. Since many single-point calculations are needed, the trade-off between accuracy and computational cost is crucial for the practical application of MD-based Raman spectra. [1] Thomas, et al. Phys. Chem. Chem. Phys. 15, 6608-6622 (2013) [2] Grumet, et al. J. Phys. Chem. C 128, 6464-6470 (2024)

HL 20.2 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility $\mu_h = 25$ $cm^2V^{-1}s^{-1}$ being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measure-

ment, the ionization energy of shallow acceptors $E_{I,S} = 137 \pm 8$ meV and deeper acceptors $E_{I,D} = 262 \pm 23$ meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.3 Tue 10:00 P3

Semiconductor membrane transfer for deterministic Circular Bragg Gratings fabrication — •Juan Nicolas Claro Rodriguez, Dennis Deutsch, Leonie Schubert, Dirk Reuter, and Klaus Joens — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn

Highly indistinguishable single photons and strongly entangled photon-pairs are fundamental for photonic quantum communication [1]. InGaAs quantum dots (QDs) grown on InP substrates using MBE deposition [2] emit in the telecom C-band, making them ideal for long-distance communication, though their brightness is limited. Embedding these QDs in hybrid Circular Bragg Gratings (CBGs) enhances photon collection efficiency and the Purcell factor, supported by a backside mirror and transparent medium configuration [3]. We present a membrane transfer method involving backside mirror growth, press-bonding, and InP substrate removal via HCl etching, enabling emitter localization and CBG integration. PL spectra are used to assess sample quality.

[1] Applied Physics Letters, 118(10), 100502. [2] AIP Advances, 13(5). [3] Journal of the Korean Physical Society, 73(10), 1502*1505.

HL 20.4 Tue 10:00 P3

Comparative Investigations of GaN/p-GaInP and p-GaInP Photocathodes: Stability and Performance in Acidic Electrolytes — •Sahar Shekarabi[1], Mohammad Amin Zare Pour[1], David Osteimer[1], Haoqing Su[2], Wentao Zhang[2], Agnieszka Paszuk[1], Wolfram Jaegermann[3], Shu Hu[2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Yale University, Department of Chemical and Environmental EngineeringNew Haven, USA — [3]Technische Universität Darmstadt, Department of Materials and Earth Sciences, Darmstadt, Germany

GaInP(100) is a widely used photoabsorber in tandem solar cells and photoelectrochemical (PEC) devices. To enhance stability against photo-induced corrosion, GaN passivation layers have been employed. This study evaluates the stability of p-GaInP/GaN and p-GaInP electrodes for solar-driven hydrogen evolution reactions (HER) in 1.0 M HClO4. Faradaic efficiency was monitored via gas chromatography during PEC, while X-ray photoelectron spectroscopy and atomic absorption spectroscopy were used to investigate surface and dissolution process conditions. The large valence band offset of around 2.0 eV at the GaN/p-GaInP interface acts as a hole barrier, reducing recombination, while conduction band alignment facilitates electron transport. The GaN passivation layer enhances stability and achieves a low onset potential of -0.5 V for HER. Surface and electronic structural changes were analyzed to understand corrosion mechanisms.

HL 20.5 Tue 10:00 P3

Characterization of surfaces of mixed semiconductor crystals — •Marsel Karmo[1] and Martin Brehm[2] — [1]Warburger Str. 100 33098 Paderborn — [2]Warburger Str. 100, 33098 Paderborn

Compositionally disordered crystals, also known as mixed-crystals, play a crucial role in semiconductor engineering. They enable the manipulation of material properties such as the band gap, which is important for opto-electronic devices like solar cells. Additionally, these crystals are used as buffer layers to mitigate strain from lattice constant mismatches between different material layers. However, accurately describing mixed crystals theoretically presents significant challenges. Due to the random occupation of atomic sites it is not possible to introduce a unit cell in other words the crystal as a whole is the unit cell. This prohibits also the use of boundary conditions. A commonly used approach to approximate mixed crystals is the Supercell Method (SCM), which employs a large, unit cell with random atomic site occupations. While this method approximates a mixed crystal, it is limited by computational resources. Another approach is the Virtual Crystal Approximation (VCA), which replaces the mixed crystal with an analytically averaged system. This method reduces the computational effort by using a smaller unit cell but may overlook local atomic environments, potentially limiting its ability to capture certain physical properties. In this work, we compare these two methods, VCA and SCM within the Vienna Ab Initio Simulation Package (VASP) to evaluate their performance in calculating the electronic structure and surface formation energy.

HL 20.6 Tue 10:00 P3

Photoelectrochemical characterisation of InGaN/GaN nanowire arrays — •Genrietta Steingelb[1], Hannah Nell[1], Rudolfo Hötzel[1], Ruben Neelissen[1], Stephan Figge[1], Tim Grieb[1], Florian Krause[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them ideal candidates for use as electrochemical biosensors [1]. In this work, we present a detection mechanism that combines simultaneous photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, allowing sensitive and selective detection of redox-active biomolecules. However, the performance of the NW photoelectrode is limited by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly caused by unpassivated surface states. The deposition of ultrathin metal oxide films is a possibility to suppress such effects. The influence of surface coatings on sensor properties was analysed through photoelectrochemical characterisation, with and without metal oxide coatings. This analysis highlights how surface modifications affect sensor performance for the detection of redox-active molecules in complex biochemical environments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003).

HL 20.7 Tue 10:00 P3

Impact of Surface States on the Performance and Stability of AlGaAs/GaAs HEMT Structures — •Vincent Leon Spreter[1,2], Selma Delic[1,2], Xuelin Jin[1,2], Nils von den Driesch[1], Christoph Krause[1], Detlev Grützmacher[1,2], and Beata Kardynal[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, RWTH, 52074 Aachen, Germany

Electrostatic gating is commonly used to define single-electron quantum dots (QDs) in two-dimensional electron gases, such as those in GaAs/AlGaAs heterostructures. It can also be used to tune the electronic states of epitaxial quantum dots. For the use for quantum information processing applications, gated devices must maintain a stable working point over long time.

In our contribution, we investigate the effect of surface preparation of GaAs/AlGaAs heterostructure on the long-term stability of gates on the example of split-gate devices. In addition, we explore the use of passivation layers to mitigate the effects of dangling bonds associated with surface states. We discuss the processing of devices with AlOx passivation and action of electrostatic gates on device performance, offering insights into its potential for optimizing GaAs-based optoelectronic devices.

HL 20.8 Tue 10:00 P3

Low-temperature RAS of MOVPE-prepared Si(100) surfaces — •Kai Daniel Hanke[1], Max Grossmann[2], Chris Y. Bohlemann[1], Mohammad Amin Zare Pour[1], Paszuk Agnieszka[1], Runge Erich[2], and Hannappel Thomas[1] — [1]1Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]2Technische Universität Ilmenau, Theoretical Physics I, Ilmenau, Germany

Recent studies have shown that As-modified Si(100)-(2 x 1) surfaces prepared in a MOCVD environment exhibit asymmetric hydrogen-passivated Si-As dimers as dominating surface motif, in contrast to the previously assumed symmetric As dimers. Due to the importance of this surface for subsequent nucleation of III-V materials, such as GaP, for high-efficiency solar cell structures, we have performed low-temperature reflection anisotropy spectroscopy measurements, which are extremely surface sensitive, in combination with density functional theory and many-body perturbation theory calculations. We also performed X-ray photoelectron spectroscopy and low-energy electron diffraction measurements for a detailed understanding of the structure and electronic properties of this surface. Our method seeks to improve knowledge of the spectral properties of semiconductor surfaces by combining theoretical understanding with experimental data to understand the complex variables that influence RAS spectra.

HL 20.9 Tue 10:00 P3

Optimization of GaSb(100) Substrate Preparation for MBE Growth of GaSb Layers — •Peter Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany

The preparation of epi-ready substrates for MBE growth typically involves degassing and oxide removal. The latter is often done by thermal processes, resulting in rough interfaces that are associated with pyramidal defects (PDs) in GaSb layers grown on GaSb(100) substrates [1].
This study aims to optimize GaSb substrate preparation and buffer layer growth to reduce PD formation.
We compare standard thermal oxide desorption to methods proposed in the literature, such as Ga-assisted oxide removal [2] and the insertion of an AlAsSb layer into the buffer layer [1].
Using photoluminescence spectroscopy (PL) mapping, we assess quantum well and buffer layer luminescence as indicators of material quality. Additionally, we analyze the surface morphology with atomic force microscopy (AFM), focusing on the properties of pyramidal defects.

[1] Murray, Lee M., et al. *J. Vac. Sci. Technol. B* **31.3** (2013).
[2] Mathews, Sen, et al. *J. Vac. Sci. Technol. B* **35.2** (2017).

HL 20.10 Tue 10:00 P3

Passivation Protection Layers for Highly efficient Multi-Absorber Devices for Photoelectrochemical Solar Fuel Production — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Jennifer Velázquez Rojas[3], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]Paszuk Group, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

In photoelectrochemical cells with the highest solar-to-hydrogen conversion efficiencies, the heterointerface between a III-V top layer and a metal oxide protection layer should be optimized to minimize charge carrier losses. Using photoemission spectroscopy, we study the TiO_2/InP(100) heterointerface as a function of InP surface preparation and Ti precursor.

InP(100) substrates were prepared with either a well-ordered, phosphorus-terminated surface in a metal-organic chemical vapor deposition (MOCVD) reactor or with a thin oxide layer. TiO_2 was deposited via atomic layer deposition (ALD) using either titanium tetrachloride ($TiCl_4$) or titanium isopropoxide (TTIP) as the Ti precursor, along with water as the co-reactant.

Depending on the Ti precursor and the InP surface preparation, we observed either a nucleation delay or acceleration and differences in the band alignment. Layers grown with the TTIP precursor showed the presence of Ti^{3+} states, which may act as trap centers.

HL 20.11 Tue 10:00 P3

Characterization of Arsenic- and Antimony Containing Heterostructures Grown by Molecular Beam Epitaxy — •Max H. W. Ziehfreund[1], Peter F. Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[1,2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik der Ruhr-Universität Bochum, 44801 Bochum, NRW, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, NRW, Germany

This study focuses on the investigation of the surface morphology of various arsenic- and antimony-containing semiconductor heterostructures grown by molecular beam epitaxy. The objective is to optimize the growth parameters used in fabrication and to gain a better understanding of the underlying growth process. The characterization methods developed and approved for GaAs-based heterostructures are applied to GaSb-heterostructures. The primary methods employed are photoluminescence spectroscopy and atomic force microscopy. It was possible to examine the influence of various parameters, such as the antimony flux used during growth on the epitaxial quality of the grown layers and collect valuable experience for defect-free growth of arsenic- and antimony-containing heterostructures.

HL 20.12 Tue 10:00 P3

High Resolution Temperature Mapping of GaSb Wafers during MBE Growth — •Timo A. Kurschat[1], Sascha R. Valentin[1], Peter Zajac[2], Rainer Krage[1], and Andreas D. Wieck[2] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, D-44143 Dortmund — [2]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44801 Bochum

The substrate temperature is one of the most important parameters during MBE growth. Thermocouples and pyrometers, as well as more advanced techniques, measure only a single spot on the wafer at a time. Knowing the temperature distribution allows to optimize the growth parameters from just a single grown sample.

To obtain high-resolution thermal maps we use a commercial SLR camera with its infrared filter removed. The sensor is sensitive up to a wavelength of about 1000 nm and can therefore be used as a high resolution pyrometer. Without substrate rotation and 10 s exposure time, measurements can be made down to $T_S = 400\,°C$. With rotation enabled and a reduced exposure time of 0.25 s, it is still possible to obtain images at the growth temperature of $T_S = 680\,°C$.

Images of quarter 2-inch GaSb wafers show differences of more than 20 K between the center and the corners. The effect of a washer was investigated with this method, which is a ring placed at the backside of the wafer to improve its temperature uniformity. The temperature differences also effect the photoluminescence intensity of a quantum well grown on the wafer.

HL 20.13 Tue 10:00 P3

Raman spectroscopy on MBE grown III-V semiconductors heterostructures — •Arijit Chakraborty[1], Yiteng Zhang[1], Tom Fandrich[1], Doaa Abdelbarey[1], Tom Rakow[1], Krupali Dobariya[1], Sulabh Shrestha[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover, Institute for Solid State Physics, Hannover, Germany — [2]Leibniz Universität Hannover, Laboratorium for Nano- und Quantum Engineering, Hannover, Germany

We present micro-Raman spectroscopic measurements on molecular beam epitaxy (MBE) grown semiconductors heterostructures, and quantum dots. This technique offers unique insights into the vibrational modes, crystal structure, strain, alloying effects and defects of grown semiconductor structures, making it invaluable for the optimization of MBE processes. The Raman results for the relaxed material have been interpreted in the framework of the modified random element isodisplacement theory considering different vibrational modes of the lattice with changing compositional range. Optical-phonon deformation potentials have been successfully used to fit the different vibrational phonon frequencies in strained layers of semiconductors. Using comparable theoretical models, a substantial compositional dependency with phononic vibrations is found and established. Disordered activated vibrational modes are investigated for layers produced on various substrates. An analogous conclusion with the peak shift in photoluminescence spectra is reached by analyzing the Raman spectra of herostructures grown on InP-based substrates.

HL 20.14 Tue 10:00 P3

Copper tin oxide: an amorphous, bipolar, ternary oxide system with tunable electrical and optical properties — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics

Copper oxide (CuO) is one of the most studied p-type semiconducting metal oxides [1]. Tin oxide (SnO_2) features high transparency in the visible range, high n-type electrical conductivity and non-toxicity [2]. Due to mismatching crystal structures of CuO and SnO_2 (and their other oxidation states) an amorphous alloy, copper tin oxide (CTO), can form when combining these materials. Depending on growth pressure and cation composition the material can be p-type [1] or n-type making it a promising candidate for complementary amorphous devices. In this work, we investigated physical properties of CTO thin films, deposited by combinatorial pulsed laser deposition of segmented CuO and SnO_2 targets at room temperature and in oxygen atmosphere, as a function of cation composition and growth pressure. The resulting samples are X-ray amorphous and n-type semiconducting with mobilities up to $11\,cm^2/Vs$ for $Cu/(Cu+Sn) < 0.8$. Optical and electrical properties can be tuned by varying composition ratio and oxygen pressure. A temperature-dependent Hall effect analysis has led to the conclusion that the percolation model provides the most accurate description. For $Cu/(Cu+Sn) > 0.8$, the samples become p-type conducting and feature low mobilities.
[1] Isherwood *et al.*: J. Appl. Phys., 118, 105702, (2015)
[2] Ni *et al.*: Surface and Coating Technology, 206, 4356-4361, (2012)

HL 20.15 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility $\mu_{\mathrm{h}} = 25$ cm^{2}V^{-1}s^{-1} being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measurement, the ionization energy of shallow acceptors $E_{\mathrm{I,S}} = 137 \pm 8$ meV and deeper acceptors $E_{\mathrm{I,D}} = 262 \pm 23$ meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.16 Tue 10:00 P3

Mechanical, electronic and optical properties of $LiNbO_2$ and $NaNbO_2$ from first-principles calculations — •Frederik Schmidt and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

The layered compound $LiNbO_2$ is of interest as a superconductor and possible battery material, but its electronic and optical properties have not yet been extensively analyzed, especially in theoretical simulations. There are even fewer studies of the closely related $NaNbO_2$. In this work, we perform first-principles calculations to investigate the properties of $LiNbO_2$ and $NaNbO_2$. The elastic constants and related parameters, such as elastic moduli, are determined using density-functional theory. We show that even small biaxial strain up to $\pm 5\%$, which corresponds to common substrates like $MgAl_2O_4$ or SiC, may lead to significant changes in the electronic band structure and to a qualitative transition from a direct to an indirect band gap. Accurate results for the electronic band structure and the optical absorption spectrum are obtained from the *GW* approximation and the Bethe-Salpeter equation. We find that both the quasiparticle corrections and excitonic effects have a significant influence on the dielectric function. Good quantitative agreement with the experimentally measured absorbance and the absorption edge at 2 eV for $LiNbO_2$ is achieved only by a proper inclusion of both factors.

HL 20.17 Tue 10:00 P3

Bismuth oxyselenide (Bi2O2Se): Insights into chemical bonding and structural properties — •Sumayya Sumayya[1], Yuan Yu[1], Carl Friedrich Schon[1], Kim Dasol[1], Yueyang Yang[2], and Matthias Wuttig[1] — [1]RWTH, Aachen, Germany — [2]Tsinghua University, China

The Bismuth Oxychalcogenides (Bi2O2X, X=S, Se, Te) are potential candidates in various fields such as Thermoelectrics, Ferroelectrics, Piezoelectrics, and photodetectors due to their unique 2D layered structure containing a bismuth oxide layer and a chalcogen layer. In this family, Bi2O2Se is considered the 2D rising star for the semiconductor industry because of its high crystallographic symmetry, tunable band gap, ultra-high electron mobility, strong Shubnikov-des Haas quantum oscillations, unique defects, and excellent stability. The relationship between bonding and material properties offers a versatile platform for tailoring electronic and vibrational properties, potentially leading to improved functional characteristics. Recently, many theoretical and experimental bonding descriptors such as electron transferred and shared values, Born effective charge, electrical conductivity, optical dielectric constant, Grüneisen parameter, and Probability of Multiple events in atom probe tomography have been devised. Our study employs a combination of advanced characterization techniques and theoretical calculations to probe the nature of bonding at different length scales, from local atomic level to extended structural motifs. In the future, this model can be used for other layered materials to understand the structure-property relationship via chemical bonding.

HL 20.18 Tue 10:00 P3

Reactive Sputter Deposition and Nitrogen Modification of $CuBi_2O_4$ as Photocathode — •Dominic Rapf[1,2], Tsedenia A. Zewdie[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, D-85748 Garching, Germany

Copper bismuthate ($CuBi_2O_4$) is a ternary oxide that is of special interest for photoelectrochemical (PEC) water splitting. Unlike most transition metal oxides, which predominantly exhibit n-type conductivity, copper bismuthate is a native p-type semiconductor. [1] In addition, it has a suitable bandgap for the absorption of visible light, as well as a high photocurrent onset potential > 1 V vs. RHE. [2] These properties make $CuBi_2O_4$ highly desirable as a photocathode. This project focuses on the development of reactive co-sputter recipes to deposit copper bismuthate thin films and their structural, optical, morphological and opto-electronic analysis. In addition, we explore nitrogen incorporation to narrow the band gap of $CuBi_2O_4$ for more efficient light absorption (N:$CuBi_2O_4$). By modifying the nitrogen content in the reactive gas mixture and applying post-annealing treatments, we can tailor the level of nitrogen incorporation. On a library of N:$CuBi_2O_4$ thin films, we investigate the impact of nitrogen incorporation on optical and structural properties and assess their PEC performance.

[1] J. K. Cooper et al., Chem. Mater. 2021, 33, 3, 934–945 [2] D. Kang et al., Chem. Mater. 2016, 28, 12, 4331–4340

HL 20.19 Tue 10:00 P3

The impact of Bi and Na non-stoichiometry on the electrocaloric effect in (Na0.5Bi0.5)TiO3-BaTiO3 ceramics — •Sobhan M. Fathabad, Mohammadamin H. Kashani, Eva Kröll, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisubrg-Essen (CENIDE), University of Duisburg Essen, Essen, Germany

The electrocaloric effect (ECE) is the phenomenon where polar crystals experience a change in isothermal entropy or adiabatic temperature in response to the application or removal of an electric field. In this work, we investigate the influence of Bi and Na non-stoichiometry on the depolarization mechanism and electrocaloric effect in BaTiO3 - (Na0.5Bi0.5)TiO3 compounds at the morphotropic phase boundary. Ceramic samples were prepared using the solid-state synthesis method. The polarization hysteresis loops were measured in the temperature range from -20 °C to 200 °C and subsequently the ECE was indirectly estimated in the framework of the thermodynamic approach based on the Maxwell relation. The depolarization temperature was studied using dielectric permittivity, X-ray diffraction, and pyrocurrent analysis. Direct measurements of the ECE were conducted using a quasi-adiabatic calorimeter. It was shown that the introduced defects reduce the depolarization temperature, consequently shifting the maximum ECE towards room temperature.

HL 20.20 Tue 10:00 P3

Structure and lattice distortions of KTaO3(001) studied by LEED I-V and nc-AFM — Dominik Wrana[1,2], Marek Kuzmiak[1], Michele Reticcioli[3], Tomas Dolak[1], Florian Kraushofer[4], Michele Riva[5], Aji Alexander[1], Llorenc Albons[1], Jesus Redondo[1], Cesare Franchini[3], and •Martin Setvin[1] — [1]Charles University, Prague, Czech Republic — [2]Jagiellonian University, Krakow, Poland — [3]University of Vienna, Vienna, Austria — [4]TU Munich, Germany — [5]TU Wien, Vienna, Austria

Perovskites attract attention in many fields, yet understanding their surface structure represents a challenge. Special emphasis is focused on little lattice distortions associated with ferroelectric properties, often present in this broad class of materials. Hydroxylated KTaO3(001)-(2x1) is used here as a test case to extract the precise positions of lattice atoms by means of low energy electron diffraction (LEED) I-V, obtaining a final Pendry R-factor below 0.17. The main challenge lies in the extreme sensitivity of this surface to damage induced by the electron beam; the progressing damage is visualized at the atomic scale by noncontact atomic force microscopy (nc-AFM). Positions of lattice atoms obtained from LEED I-V analysis are used as a benchmark for a comparison with theoretical calculations performed within 30 different setups. The overall trend is that the closest match with the experiment is obtained for setups without the Hubbard U-term and with the SCAN functional

Work supported by GACR 20-21727X and MSMT LL2324.

HL 20.21 Tue 10:00 P3

Photoluminescence and photophysical properties of halide perovskite MAPbBr3 single crystal — •Liangling Wang[1,2], Francesco Vitale[2], Edwin Eobaldt[2], Thomas Alexander Zaunick[2], and Carsten Ronning[2] — [1]School of Physics and Technology, University of Jinan, Jinan 250022, P. R. China — [2]Institute of Solid State Physics, Friedrich-Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The remarkable optoelectronic properties of halide perovskite MAPbBr3 (MA=methylammonium), including near-unity photoluminescence quantum yield (PL QY), small full width at half-maximum (FWHM), tunable bandgap by mixing halide and defect tolerance, make it a compelling candidate material in solar cell, light emitting diodes (LED), photodetectors, X-ray imaging, and so on. The PL spectrum of MAPbBr3 at room temperature can be deconvoluted into two emission peaks. The major peak at 545 nm arises from band-to-band transition, while the lower energy peak at 560 nm is associated with recombination in trap states (Br vacancies) below the optical gap. Interestingly, PL enhancement of MAPbBr3 is found under certain laser irradiation, indicating that the surface defects are benefit charge carrier trapping and recombination. In order to verify the origin of the emission centers, power dependent PL, including both power increase and decrease processes, will be analyzed. Furthermore, thermal activation and excitonic effects of PL under different temperature from cryogenic temperature of liquid Helium to room temperature will be investigated.

HL 20.22 Tue 10:00 P3

Resolving temporal signatures of optical excitations in semiconductor nanostructures — •Lion Krüger, Fabian Brütting, Moritz B. Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Characteristic ultrafast signatures in the photo-induced response of nanostructured materials encode the class of optical excitations and characterize the performance for opto-electronic applications. Time-resolved visible transient absorption (TA) spectroscopy and optical pump THz probe (OPTP) spectroscopy are well-established methods for contact-free probing of ultrafast dynamics. Here, we present correlated TA-OPTP measurements performed in a setup that combines multiple probing modalities under identical excitation conditions. In particular, we present different strategies to enhance detection speed and sensitivity, enabling the disentanglement of free carrier and excitonic signatures in semiconductor nanostructures of varying dimensionality and quantum-confinement [1].

[1] Motti, Silvia G., et al. "Exciton Formation Dynamics and Band-Like Free Charge-Carrier Transport in 2D Metal Halide Perovskite Semiconductors". Advanced Functional Materials 33 (2023)

HL 20.23 Tue 10:00 P3

Characterization of the electrical properties of Bismuth doped Methylbenzylamine Lead Iodide 2D Perovskites using impedance spectroscopy — •Keito Mizukami[1,2,3], Hannes Hergert[1,3], Tim Schneider[3,4], Jan Heinrich Littmann[1,3], Satoko Fukumori[2], Philip Klement[1,3], Derck Schlettwein[3,4], Hirokazu Tada[2], Sangam Chatterjee[1,3], and Matthias T. Elm[1,3] — [1]Institute of Experimental Physics I, JLU Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan — [3]Center for Materials Research, JLU Giessen, Giessen, Germany — [4]Institute of Applied Physics, JLU Giessen, Giessen, Germany

Low-dimensional organic-inorganic perovskites offer largely tunable materials properties such as the crystal structure or the electronic band gap due to the flexibility of the incorporated building blocks. Perovskites with incorporated chiral organic molecules as the cation attract a lot of attention as they exhibit chiral properties such as chirality-induced spin selectivity or spin-polarized electron current. However, the typically low electrical conductivity hinders applications and requires appropriate doping schemes to improve the device performance. In this study, we investigate the impact of Bi substitution for Pb in methylbenzylamine bismuth lead iodide single crystals and thin films on the electric properties using impedance spectroscopy. Our objective is to get a fundamental understanding of the charge transportation and relaxation mechanism in these mixed conductors.

HL 20.24 Tue 10:00 P3

Hysteretic Piezochromism in a two-dimensional perovskite — •Paul Steeger[1], Mohammad Adnan[1], Thorsten Deilmann[2], Xiang Li[3,4], Susanne Müller[4], Katarzyna Skrzynska[5], Michael Hanfland[4], Efim Kolesnikov[3], Jutta Kösters[6], Theresa Block[6], Robert Schmidt[1], Ilya Kupenko[3,4], Carmen Sanchez-Valle[3], Vijaya Prakash[7], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Physikalisches Institut Universität Münster — [2]Institut für Festkörpertheorie Universität Münster — [3]Institute für Mineralogie Universität Münster — [4]Europäischer Synchrotron ESRF Grenoble — [5]Institute of Earth Sciences University of Silesia — [6]Institut für Anorganische und Analytische Chemie Universität Münster — [7]Department of Physics IIT Dehli

Two-dimensional inorganic-organic hybrid perovskites hold potential for application in the field of optoelectronics. One representative of this class of materials is cyclohexenyl-eythylammonium lead-iodide (CHPI). Here, we present pressure-dependent optical absorption and emission spectra of CHPI. We find a strong change of the band gap when exerting pressure on the crystal using a diamond anvil cell. In contrast to other 2D perovskites the bandgap of CHPI undergoes a full hysteresis loop under pressure. To reveal the origin of the observed phenomena, we combine our optical experiments with DFT calculations as well as X-ray diffraction measurements under high pressure. Reference: Steeger et al., Hysteretic Piezochromism in a Lead Iodide-Based Two-Dimensional Inorganic-Organic Hybrid Perovskite. JACS 146, 23205 (2024)

HL 20.25 Tue 10:00 P3

Electron and Hole polaron Formation in lead-free CsGeX3 (X=Cl,Br,I) perovskites — •Mehmet Baskurt — Chalmers University of Technology

The unique electronic properties of CsGeX3 (X = Cl, Br, I) perovskites make them promising candidates for nonlinear optical applications. The nature of charge localization must be understood to explain their physical and electronic behaviors. Here, we carry out a theoretical investigation on electron and hole polaron formation in CsGeX3. We carry out density functional theory calculations in the hybrid function level. Our results show that there is a trend in the polaron formation energies, CsGeCl3 > CsGeBr3 > CsGeI3. In particular, single electron polarons form highly favorably in all three materials, whereas single hole polarons can only be formed in CsGeCl3. Moreover, double electron polarons form energetically favorably across the series. These findings constitute a basis for understanding polaronic effects on the electronic properties of CsGeX3 perovskites and open up access to their optimization in nonlinear optical applications.

HL 21: Graphene: Electronic Structure and Excitations (joint session O/HL)

Time: Tuesday 10:30–12:15 Location: H6

HL 21.1 Tue 10:30 H6

Doping of epitaxial graphene by proximitized 2D quantum islands — •Julian Koch[1], Sergii Sologub[1,2], Chitran Ghosal[1], Dorothee Boesler[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The effects of 2D quantum islands on the transport properties of monolayer graphene/SiC(0001) were investigated by magnetotransport. Two types of adsorbates are compared, Bi(110) and Pb(111) islands with average coverages of up to 3.6 bilayers (BL) and 3 monolayers (ML), respectively. The analysis is supported by structural investigations using SPA-LEED and STM. The doping behaviour of both materials is fundamentally different. In the case of Bi, the carrier concentration determined from the SdH oscillations remains at 1×10^{13} cm^{-2} independent of the Bi coverage, although photoemission spectroscopy revealed a strong doping of the graphene by Bi [1]. This strongly indicates a highly anisotropic carrier concentration across the surface and is confirmed by a positive, temperature independent contribution to the magnetoresistivity. The Bi islands rather behave as antidots and reduce the charge carrier mobility slightly from around 2250 cm^2/(Vs) for MLG to 1920 cm^2/(Vs) at 2.4 BL Bi. In contrast, there are no signs of an anisotropic carrier concentration or mobility when Pb is adsorbed. The electron concentration increases uniformly by approximately 5×10^{11} ML^{-1}cm^{-2}. The mobility is reduced from around 1400 cm^2/(Vs) for MLG to 1200 cm^2/(Vs) at 3 ML Pb.

[1] Gierz et al. *Nano Lett.* **8**, 12, 4603 (2008)

HL 21.2 Tue 10:45 H6

Photocurrent control in a graphene-based Floquet topological insulator — •Weizhe Li[1], Daniel Lesko[1], Tobias Weitz[1], Simon Wittigschlager[1], Christian Heide[1,2], Ofer Neufeld[3], and Peter Hommelhoff[1,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel — [4]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Topological insulators offer unique opportunities for novel electronics and quantum phenomena. However, intrinsic material limitations often restrict their applications and practical implementation. A circularly-polarized laser pusle can generate topologically non-trivial non-equilibrium states known as Floquet topological insulators (FTIs) which host a variety of topological phenomena. Floquet engineering with strong optical fields opens routes to optically tunable band structures and devices for petahertz electronics.

Here we demonstrate coherent control of photocurrents in light-dressed graphene. Circularly-polarized laser pulses dress the graphene into an FTI, and phase-locked second harmonic pulses drive electrons in the FTI. This approach allows us to measure all-optical anomalous Hall currents and photocurrent circular dichroism, which put FTIs on equal footing with equilibrium topological insulators. The coherent control of photocurrents in graphene-based FTI connects optics tools to condensed matter physics.

HL 21.3 Tue 11:00 H6

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], Philip Schädlich[1], Bharti Matta[3], Philipp Rosenzweig[3], Kathrin Küster[3], Ulrich Starke[3], Thomas Seyller[1], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Two-dimensional materials such as graphene are fascinating because they combine unique mechanical and electronic properties. The next level of complexity, however, comprises the assembly of various stacked 2D materials to generate structures with desired properties. Intercalation of epitaxial graphene systems is an effective method to tailor the electronic, optical, and transport properties of graphene while keeping its honeycomb lattice on SiC. Furthermore, intercalation facilitates the synthesis of otherwise unstable 2D layers. A wide range of elements have been used as intercalants below a graphene sheet, forming often well-defined heterobilayers with different functionalities. In particular, intercalation of heavy elements such as Pb and Bi are specially promising since they can introduce additional effects such as spin-orbit coupling to the electron gas of graphene and Rashba spin polarization. Using first-principles methods, we investigate the modifications in the electronic structure of epitaxial graphene due to proximity effects induced by intercalation.

HL 21.4 Tue 11:15 H6

Accelerated Exploration of Defective Graphene Superstructures — •Benedict Saunders[1], Lukas Hörmann[1,2], and Reinhard Maurer[1,2] — [1]Department of Chemistry, University of Warwick, Coventry — [2]Department of Physics, University of Warwick, Coventry

Graphene has been meticulously studied due to its remarkable mechanical, electrical, and thermal properties. It is well documented that introducing various dopants and defects to the lattice can be used to tune the material's properties for a specific application, such as in electronics, sensors, or catalysis. In order to design graphene with specific properties, one must achieve precise control over the composition and concentration of defects. This requires a fundamental understanding of the stability of defects and their interaction in a given superstructure. We present a comprehensive method for exploring the configurational space of defective 2D superstructures. We have extended the SAMPLE structure search code to defects in 2D materials. SAMPLE uses Bayesian learning based on sparse Density Functional Theory data for structure exploration. We show the capabilities of our approach for a proof-of-principle application on free-standing graphene with heteroatom defects. Finally, we use the SAMPLE code to gain physical insight into the interactions between these defects, paving the way for effective and rational growth models of topologically designed defective graphene.

HL 21.5 Tue 11:30 H6

Polymorphism of a two-dimensional Pb layer underneath charge neutral graphene on SiC — •Markus Gruschwitz, Sergii Sologub, Zamin Mamiyev, Chitran Ghosal, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Germany

Since the first studies on graphene, researchers strive to implement its unique properties in industrial relevant processes. The intercalation of epitaxially grown buffer layers on SiC results in high quality, quasi-freestanding graphene, which allows the electronic properties to be modified by varying the intercalants and their arrangement. Pb recently sparked a great interest by reliably providing almost perfectly charge neutral graphene. The Pb layer effectively screens the substrate induced doping. In a novel approach using differential phase contrast in cross-sectional scanning transmission electron microscopy we reveal their vertical charge density distribution. Surprisingly, the charge neutrality is robust against variations in the Pb interface reconstruction. Depending on the preparation, a Pb monolayer often reconstructed in two coexisting phases, the so-called stripe [1] or bubble [2] phase. Intercalated multilayers reveal a similar striped phase arising from two twisted plumbene layers [3]. Here we combine structural investigations by scanning tunneling microscopy and high-resolution low-energy electron diffraction in a model of flexibly arranged grain boundaries releasing lattice mismatch stress.

[1] Materials 14, 7706 (2021), [2] Adv. Mater. Interfaces 10, 2300471 (2023), [3] Phys. Rev. Lett. 129, 116802 (2022)

HL 21.6 Tue 11:45 H6

Facet-dependent growth and properties of graphene on Al_2O_3 surfaces from first principles — •Armin Sahinovic and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The direct growth of graphene on functional substrates such as sapphire (Al_2O_3) enables the use in optoelectronic devices without the necessity of sample transfer. We explore the role of the surface orientation of Al_2O_3 on the growth of graphene [1] using density functional theory. The stoichiometric terminations are identified as the most stable surface terminations of the C-, R- and A-plane facets in the framework of *ab initio* thermodynamics. Next, we consider the adsorption of carbon atoms on the different surface facets, varying their position and concentration. The adsorption energy shows the weakest binding

at the R-plane and the most favorable at the A-plane. We associate this with the more unsaturated oxygen bonds at the A-plane compared to the R- and C-plane. Furthermore, we explore the graphene - Al_2O_3 interaction and its impact on the electronic properties of graphene. Our results provide a deeper understanding of the role of the surface facets of the substrate in the scalable graphene growth on Al_2O_3.

Funding by GRK2803 2D-MATURE (Project P4) and computational time at the supercomputers MagnitUDE and AmplitUDE are gratefully acknowledged

[1] Y. Ueda et al., Appl. Phys. Lett. 1, 115 (1), 013103 (2019)

HL 21.7 Tue 12:00 H6

Enhanced light-matter interactions via Sn nanoislands on epitaxial graphene — •Zamin Mamiyev, Narmina Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Surface-enhanced Raman scattering (SERS) is an advanced technique for coupling light into quasiparticle excitations in low-dimensional materials, offering promising applications in trace detection, enhanced light-matter interactions, photonic energy harvesting, and catalytic processes. Recent studies in this field have focused on integrating noble metal nanostructures with graphene.

In this study, we investigate a novel SERS platform utilizing tin (Sn) nanoislands to enhance graphene Raman signals by up to two orders of magnitude. We examine the SERS performance on Sn-intercalated charge-neutral and intrinsically doped epitaxial monolayer graphene (MLG) on SiC(0001). The increase in the Raman cross-section and enhanced intensity is accompanied by spectral shifts, which may be correlated with the localized surface plasmons (LSPs) of Sn nanoislands as well as dynamic charge transfer between the Sn particles and graphene. This dynamic charge redistribution, primarily determined by the doping concentration and interface interactions, enables control over the SERS response. Additionally, plasmonic and thermalization-induced carrier density propagation across μm ranges indicates efficient coupling between localized and propagating plasmons.

[1] Z. Mamiyev and C. Tegenkamp, 2D Materials. 11, 025013 (2024)
[2] Z. Mamiyev and C. Tegenkamp, Surf. & Int. 34, 102304 (2022)

HL 22: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

HL 22.1 Tue 10:30 H8

Line-moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) — •Romana Ganser, Muthu P. T. Masilamani, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

We present angle-resolved photoemission spectroscopy (ARPES) measurements on tunable one-dimensional moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) [1]. In this model system, the moiré structure can be tuned almost continuously in contrast to hardly controllable twist angles in bilayer van-der-Waals heterostructures [2]. We experimentally observe moiré minibands and band gaps of 120 - 170 meV suggesting sizable superlattice potentials. By comparing the experimental data to simple model calculations, we analyze the local character of the potential. This provides important information of interface hybridization effects on the band structure, which may not be limited to the system at hand but rather a broad range of moiré interfaces.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020).
[2] Lisi, S. et al. Nat. Phys. 17, 189-193 (2021).

HL 22.2 Tue 10:45 H8

Photoemission Time Scale Determination: the Effect of Crystal Dimensionality and Electronic Correlation — •Fei Guo[1], Dmitrii Usanov[2], Eduardo B. Guedes[2], Mauro Fanciulli[3], Arnaud Magrez[1], Michele Puppin[1], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, 95031, France

Spin polarization of photoelectrons from spin-degenerate dispersive initial states originates from the interference of multiple photoemission channels, measuring the spin polarization with spin- and angle-resolved photoemission spectroscopy (SARPES) allows the estimation of the phases of the interfering channels, and hence the Eisenbud-Wigner-Smith (EWS) time delay of photoemission, which is the amount of time required by the photoelectron to evolve into a free particle final state. While not directly measurable for solid-state photoemission, this time scale has been measured for gaseous photoionization, which is generally in the attosecond (10^-18s) range.

We present investigations with multiple materials of different properties, and by comparing with previous studies, we propose a relationship between the EWS time delay, electronic correlation mechanism, and dimensionality.

HL 22.3 Tue 11:00 H8

Disorder effects in the Band Structure of Transition Metal Dichalcogenide alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W) — •Sarath Sasi[1], Aki Pulkkinen[1], Laurent Nicolaï[1], Raphaël Salazar[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

Recent advances in materials synthesis have enabled the creation of 2D TMDC alloys, which offer unique opportunities for tailoring electronic and optoelectronic properties to meet diverse application demands.[1].This study investigates the band structure evolution of $A_xB_{1-x}Se_2$ alloys (A, B = Cr, Mo, W) across varying composition fractions (x). Using the Coherent Potential Approximation (CPA)[2], which accurately models scattering in disordered systems, theoretical calculations were performed with the *SPR-KKR* package[3]. Results reveal that some of the TMDC alloys maintain their band structures without significant disorder effects. Angle-Resolved Photoemission Spectroscopy (ARPES) measurements align closely with one-step model photoemission calculations, confirming theoretical predictions. These insights provide a foundation for tailoring electronic properties, advancing their applicability in next-generation devices.

[1] Zhou, J., Lin, J., Huang, X., et al. Nature, 556, 355-359 (2018).
[2] Soven, P., Phys. Rev., 156, 809(1967).
[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

HL 22.4 Tue 11:15 H8

Unveiling Doping-Induced Electronic Modifications in Antiferromagnetic MPS_3 van der Waals Materials — •Till Willershausen[1], Jonah Elias Nitschke[1], Patrick Merisescu[2], David Janas[1], Lasse Sternemann[1], Michele Capra[1], Mira Arndt[1], Valentin Mischke[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Bath University

Antiferromagnetic van der Waals (vdW) materials, with scalability to monolayer thickness, semiconducting properties, and intrinsic antiferromagnetic ordering, hold promise for spintronic and quantum technology applications. We investigate alkali metal doping effects on the MPS_3 family (M = Mn, Ni, Co, Fe) of 2D antiferromagnetic vdW materials, revealing doping-induced changes in their electronic structure. X-ray Photoelectron Spectroscopy (XPS) shows shifts in oxidation states in $NiPS_3$, $CoPS_3$, and $FePS_3$, while $MnPS_3$ displays no significant changes, indicating distinct charge transfer. Further investigation with Angle-Resolved Photoelectron Spectroscopy (ARPES) reveals new alkali-metal induced bands appearing above the previous valence band maximum. This analysis highlights doping-induced modifications and contrasts in transition metal behavior in MPS_3, providing insights into doping mechanisms and electronic tunability.

HL 22.5 Tue 11:30 H8

Enhanced electron-phonon coupling in few-layer $MoTe_2$ from micro-ARPES — •Thomas P. van Waas[1], Julia Issing[2], Marco Gibertini[3], Christophe Berthod[2], Anna Tamai[2], Felix Baumberger[2,4], and Samuel Poncé[1,5] — [1]European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium —

[2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland — [5]WEL Research Institute, Belgium

Bulk orthorhombic T_d-$MoTe_2$ is a type-II Weyl semimetal with a superconducting critical temperature of $T_c = 0.1$ K. Transport measurements show a monotonic increase in T_c as the thickness of multilayer $MoTe_2$ is reduced, reaching $T_c = 7.6$ K in the monolayer. We investigate photoemission kinks in the electron pocket of exfoliated mono-bi-, and trilayer $MoTe_2$ from micro-focused angle-resolved photoemission spectroscopy. We use a custom code to quantify the electron self-energy $\Sigma_n(E)$ for a parabolic non-interacting dispersion, and obtain from $\Sigma_n(E)$ the Eliashberg spectral function $\alpha^2F_n(\omega)$ using the maximum entropy method. We find two dominant phonon modes in $\alpha^2F_n(\omega)$ for the mono- and trilayer, with a large enhancement of the lower-frequency phonon mode in the former. We also provide tentative results for the bilayer, where quantification is more challenging due to a small splitting of the electronic bands.

HL 22.6 Tue 11:45 H8

Electronic structure of V-doped WSe_2 — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics represents a promising and energy-efficient alternative to conventional electronics, with significant potential applications, e.g., in areas such as classical and quantum computing. The vanadium-doped layered transition metal dichalcogenide 2H-WSe_2 is a promising candidate to fulfill the desired properties as a room-temperature magnetic semiconductor with gating tunability. Here, we present a comprehensive electronic structure study of chemical vapor transport-grown pristine and V-doped WSe_2 by soft X-ray, VUV and 11eV-laser ARPES, highlighting the influence of a low V doping concentration on the electronic structure of WSe_2.

HL 22.7 Tue 12:00 H8

Unraveling magnetic ordering in a van der Waals correlated material — Tommaso Pincelli[1,2], •Tania Mukherjee[1,2], Lawson Lloyd[2], Shuo Dong[2,3], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], and Ralph Ernstorfer[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society, 14195 Berlin, Germany — [3]Beijing National Laboratory for Condensed Matter Physics, China

Layered van der Waals (vdW) materials offer a compelling platform to investigate various emergent quantum properties in low dimensions. Fe_3GeTe_2 (FGT), a vdW ferromagnetic metal, is well-known for exhibiting exotic phenomena, ranging from skyrmion formation to heavy fermion behavior. However, an understanding of the magnetic ordering, a key feature for spintronic applications, still remains elusive in this material. In particular, the interplay of both local magnetic moments and an itinerant mechanism in the formation of ferromagnetic ordering in FGT, a non-f-electron correlated system, remains to be clarified. Using time- and angle-resolved photoemission spectroscopy (trARPES) and first-principles calculations, we provide evidence for an ordering mechanism in FGT by observing a pronounced reduction in the Stoner exchange gap. This stands in contrast to earlier temperature-dependent ARPES studies of the electronic structure of FGT, which favored a localized excitation model over the weak-coupling itinerant picture. We also observe the impact of phononic excitations which further confirm our findings.

HL 22.8 Tue 12:15 H8

Spin structure of the unoccupied surface state at AgTe/Ag(111) — •Carolin Benfer, Marcel Holtmann, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

The AgTe/Ag(111) surface alloy has recently been investigated as a model system for the role of orbital angular momentum in the formation of spin effects in the electronic structure [1]. Two p-like surface states were detected in ARPES measurements, one shows a Rashba-type spin splitting, while the other one does not. This behavior is attributed to the symmetries of the orbital wave functions of the electrons. For the unoccupied states a third surface state has been predicted. Following the symmetry arguments given in [1], a Rashba-type spin splitting of the state is expected.

We use inverse photoemission (IPE) to directly study the unoccupied state of the surface alloy. Low-energy electron diffraction and scanning tunneling microscopy measurements confirm a homogeneous monolayer film of the surface alloy, which is growing in a honeycomb structure. Angle-resolved IPE measurements detect the predicted surface state with free electron-like dispersion. Spin-resolved IPE measurements reveal a Rashba-type spin structure.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

HL 22.9 Tue 12:30 H8

Orbital mixing as key mechanism for ferromagnetism in van der Waals CrI3 — •Alessandro De Vita[1,2], Srdjan Stavrič[3], Roberto Sant[4], Nicholas B. Brookes[4], Giancarlo Panaccione[5], Silvia Picozzi[3], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17 Juni 135, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]Consiglio Nazionale delle Ricerche CNR-SPIN, c/o Università degli Studi G. D'Annunzio, 66100 Chieti, Italy — [4]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [5]Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, km 163.5, I-34149 Trieste, Italy

Van der Waals ferromagnets constitute a versatile platform where exotic quantum states can be realized; among them, CrI3 is a prototypical and widely studied 2D ferromagnet, with promising applications in spin- and orbitronics. Despite that, key information on its electronic occupation and stabilization of the magnetic configuration are missing. By means of complementary absorption and photoemission spectroscopies, and density functional theory calculations, we give a description of the orbital character of bulk CrI3, and demonstrate that the emergence of ferromagnetism in this material is underpinned by the orbital mixing between I p and Cr eg states. Our results have clear impact on the understanding of how microscopic interactions at the orbital level stabilize ordered states in van der Waals ferromagnets.

HL 22.10 Tue 12:45 H8

Resonant Photoemission Studies of Transition Metal Sulfides and Selenides — •Yashasvi Mehra[1,2,3], Samuel Beaulieu[4], Mauro Faniculli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Aki I.O. Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Universite de Bordeaux CNRS CEA, CELIA, UMR5107, F33405 Talence, France

By performing resonant ARPES measurements and SPR-KKR photoemission calculations on Transition Metal Selenide, Sulfide and the Vanadium intercalated NbS2 systems, we study the interplay between different decay mechanisms in resonant conditions, radiation-less Raman Auger and Classical Auger emissions. Through a method proposed by Cini and Sawatzky we can determine the on-site Coulomb interaction per element in some cases. On the theoretical front the calculations are performed using the SPR-KKR method, which is based on one-step model, that incorporates the effect of all matrix elements which accounts for the photoemission process. Furthermore, we analyze calculated ARPES, XAS, element and orbital resolved band structure underlining agreement with experimental results and helping with its interpretation.

HL 23: Quantum Dots and Wires: Transport (joint session HL/TT)

Time: Tuesday 11:15–13:00 Location: H13

HL 23.1 Tue 11:15 H13

Transport properties of quantum dots for single-electron pumps — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Frank Hohls, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, 31668 Braunschweig, Germany

A single-electron pump (SEP) is a device emitting a well-defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e, this results in a current of $I = nef$. Since the revision of the SI system, the elementary charge e hereby is an exact value, so that SEPs provide a suitable basis for a quantum current standard. The accuracy of this current is directly related to erroneous cycles, where the emitted number of electrons deviates from n. Our SEP devices are based on electrostatically defined quantum dots in GaAs/AlGaAs two-dimensional electron gases. In such devices, the tunnel barriers as well as the energy levels are controllable via gate voltages. Based on multiple quantum dot devices we here investigate relations between transport properties and SEP operation characteristics.

HL 23.2 Tue 11:30 H13

Non-Markovian higher-order electron pump: improvement of efficiency — •Lukas Litzba, Jürgen König, and Nikodem Szpak — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany

We consider an electron pump that consists of a non–interacting quantum dot and electron baths. Our pumping setup utilizes only higher–order tunneling processes, which are purely quantum mechanical and have no classical analog. In order to study higher order tunneling–mechanism and non–Markovian effects, we extend the exact Heisenberg equation and the Laplace transform technique to time–dependent Hamiltonians and apply this technique to our model. Thereby, we identify parameter ranges which lead to a significant increase of the current flowing through the quantum dot and an improvement of the energetic efficiency of these processes.

HL 23.3 Tue 11:45 H13

Fast Machine-Learning assisted characterisation of current quantisation — •Wang Ngai Wong[1], Yannic Rath[1], Nikolaos Schoinas[1], Shota Norimoto[1], Masaya Kataoka[1], Alessandro Rossi[1,2], and Ivan Runngger[1,3] — [1]National Physical Laboratory, Teddington, TW11 0LW, UK — [2]Department of Physics, SUPA, University of Strathclyde, Glasgow G4 0NG, UK — [3]Department of Computer Science, Royal Holloway, University of London, Egham, TW20 0EX, UK

Characterisation of single-electron pumps (SEPs) has long been bottlenecked by the process of fine-tuning measurement parameters to study their novel properties. This limits potential experimental parameters to those that can remain static throughout the fine-tuning process. We demonstrate a novel method assisted by machine learning which has led to an eightfold speedup in the measurement process (see Appl. Phys. Lett. 125, 124001 (2024)), and in so doing opens the door to further characterisation experiments which are impossible using conventional methods. Our method is based around an active learning cycle to navigate the information landscape of the gate voltage parameter space, while also significantly reducing the number of measurement points required. This is paired with a post-processing approach which allows us to accurately predict and characterise the small operational regimes significantly more efficiently than conventional sweeps across the parameter space. We exploit the framework to characterise the behaviour of multiplexed GaAs multi-pump devices across a range of magnetic fields.

HL 23.4 Tue 12:00 H13

Novel Mixed-Dimensional Reconfigurable Field Effect Transistors — •Sayantan Ghosh[1,2], Muhammad Bilal Khan[1], Phanish Chava[1], Kenji Watanabe[3], Takashi Taniguchi[3], Slawomir Prucnal[1], René Hübner[1], Thomas Mikolajick[2], Artur Erbe[1,2], and Yordan M Georgiev[1,4] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]National institute for Material Science, Tsukuba, Japan — [4]Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria

The limitations of CMOS downscaling drive the exploration of alternative device concepts like reconfigurable FETs (RFETs), which can dynamically switch between n- and p-polarity through electrostatic gating. This work introduces a novel mixed-dimensional RFET utilizing 1D silicon (Si) nanowires combined with 2D hexagonal boron nitride (hBN) as a dielectric and encapsulating layer. hBN*s insulating properties, chemical stability, and absence of dangling bonds make it ideal for its use as a dielectric in 1D electronics. The RFET fabrication employs electron beam lithography, reactive ion etching, and flash lamp annealing for precise silicide formation. Mechanically exfoliated hBN flakes (5-10 nm) were integrated using dry stamping transfer, with thickness characterized by microscopy techniques. Device characterization reveals improved subthreshold swing, on-current, and ION/IOFF ratio due to hBN*s 2D passivation, highlighting its potential for advanced nanowire-based RFET architectures.

HL 23.5 Tue 12:15 H13

Kondo effect for half-filling of the third shell of a quantum dot — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany

In this work, we investigate the electrical transport in the third shell [1] of a gate-defined GaAs quantum dot. The exact number of electrons in the quantum dot (N_e) is determined using a quantum point contact as a sensitive charge detector, detecting single-electrons tunneling through the system [2]. N_e is varied by changing the applied gate voltage.

The addition energy E_c for N_e = 7 - 11 shows a triangular behavior with a maximum at half-filling of the shell. This observed behavior is described analytically with Hund's rule exchange interaction. Besides, for successive numbers of electrons occupying the quantum dot N_e = 7 to 11, a Zero-bias anomaly (ZBA) characteristic for the Kondo effect is observed [3]. The width of the ZBA exhibits a triangular behavior, with a maximum at N_e = 9, similar to E_c. The broadening of the ZBA is attributed to the contribution of the Kondo resonance as well as Hund's satellite peaks, originating from the degenerate orbitals observed in the spectral function.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64, 701-736 (2001).
[2] T. Wagner, et. al., Nat. Phys.15, 330-334 (2019).
[3] J. Schmid, et. al., Phys. Rev. Lett. 84, 5824 (2000).

HL 23.6 Tue 12:30 H13

Beyond full counting statistics and Langevin theory: The quantum polyspectra approach to multi-detector measurements — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, Germany

The quantum polyspectra approach to quantum measurements has recently been shown to cover the full range between weak and strong quantum measurements [1 - 3]. It provides thus a more general approach to quantum measurements than the full counting statistics used in nano-electronics or the Langevin-approach used in spin noise spectroscopy. This approach draws its strength from comparing higher order spectra of the measurement record with model spectra calculated from quantum expressions that are calculated on the level of a Lindblad master equation. Here, we generalize the polyspectra approach to include the case of the simultaneous measurements of more than one quantity of a quantum system. The approach regards measurement induced damping, measurement backaction, and the quantum Zeno effect. We give a few examples of multi-detector polyspectra that were calculated by a multi-detector extension of our SignalSnap and QuantumCatch library [4, 5].

[1] Hägele et al., PRB 98, 205143 (2018)
[2] Sifft et al., PRR 3, 033123 (2021)
[3] Sifft et al., PRA 109, 062210 (2024)
[4] https://github.com/MarkusSifft/SignalSnap
[5] https://github.com/MarkusSifft/QuantumCatch

HL 23.7 Tue 12:45 H13

Revealing Hidden States in Quantum Dot Array Dynamics: Quantum Polyspectra Versus Waiting Time Analysis — •Markus Sifft[1], Johannes C. Bayer[2], Daniel Hägele[1], and Rolf J. Haug[2] — [1]Faculty of Physics and Astronomy, Ruhr University Bochum, GER — [2]Institute of Solid State Physics, Leibniz Universität Hannover, GER

We show how by virtue of the recently introduced quantum polyspectral analysis of transport measurements [1,2], the complex transport measurements of multi-electron QD systems can be analyzed. This method directly relates higher-order temporal correlations of a raw quantum point contact (QPC) current measurement to the Liouvillian of the measured quantum system. By applying this method to a two-electron double QD system, we uncover dynamics between singlet and triplet states, indistinguishable in the QPC current, without requiring the identification of quantum jumps or prior assumptions about the number of quantum states involved. Our findings demonstrate that system models in such cases of hidden dynamics are inherently non-unique. Furthermore, we compare our method to a traditional analysis via the waiting-time distribution. Our method achieves parameter estimates with up to 50% lower errors, while also being applicable in scenarios with low signal-to-noise, where traditional counting methods falter. Our approach challenges previous assumptions and models, offering a more nuanced understanding of QD dynamics and paving the way for the optimization of quantum devices. [1] Hägele et al., PRB 98, 205143 (2018), [2] Sifft et al., PRR 3, 033123 (2021)

HL 24: Thermal Properties

Time: Tuesday 12:15–13:00 Location: H14

HL 24.1 Tue 12:15 H14

Combined optical and thermal characterization of III-nitride membranes by microphotoluminescence and Raman thermometry — •Gordon Callsen[1], Mahmoud Elhajhasan[1], Julian Themann[1], Katharina Dudde[1], Guillaume Würsch[1], Jean-François Carlin[2], Raphaël Butté[2], Nicolas Grandjean[2], Nakib Haider Protik[3], and Giuseppe Romano[4] — [1]Universität Bremen, Germany — [2]EPFL, Lausanne, Switzerland — [3]HU Berlin, Germany — [4]MIT-IBM Watson AI Lab, Cambridge, USA

We present the optical and thermal analysis of photonic III-nitride membranes, which provides novel insights into the physics of thermal transport on the micrometer scale [1]. By combining Raman thermometry (RT) with μPL spectroscopy, we demonstrate a non-invasive approach to extract the thermal conductivity κ. This analysis shows that even at 295 K one can still observe quasi-ballistic phonon transport in GaN, which challenges commonly applied models building on purely diffusive transport. Our membranes are made from c-plane GaN and comprise $In_xGa_{1-x}N$ (e.g., x = 0.15) quantum wells that already served as an active medium in various nanolasers [2]. The material is either grown on silicon or sapphire and is subsequently underetched, yielding freestanding structures. On such samples we perform μ-RT, either based on one-laser RT or spatially resolved two-laser RT. The latter is key to our thermal imaging, representing a significant step towards non-invasive and quantitative thermometry on photonic membranes. [1] M. Elhajhasan et al., PRB 108, 235313 (2023) [2] S. T. Jagsch et al., Nat. Commun. 9, 564 (2018)

HL 24.2 Tue 12:30 H14

Impact of AlGaAs interlayers on the thermal conductivity of GaAs micropillars — •Guillaume Würsch[1], Ching-Wen Shih[2], Mahmoud Elhajhasan[1], Katharina Dudde[1], Imad Limame[2], Stefan Reitzenstein[2], and Gordon Callsen[1] — [1]Institut für Festkörperphysik, Universität Bremen, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany

First measurements of coherent heat conduction in semiconductor superlattices (SL) were reported over a decade ago. Interestingly, such an effect that is based on phonon interference can already be observed at room temperature, which sparks interest in measuring and controlling most fundamental phonon parameters like their mean free path l_{mfp} and wavelength λ_{therm}.Observing the effects of phonon interference in SLs can be challenging, because material stacks with superb crystalline quality and interfaces is required. In this work, we follow a step-by-step approach, meaning that we analyse GaAs micropillars (diameter: 0.5 - 2 μm) with a rising number (0 - 7) of $Al_{0.8}Ga_{0.2}As$ interlayers. A thin layer of gold on top of these structures enables the measurement of the thermal conductivity κ via the frequency-domain thermal reflection (FDTR) technique, which is complementary to the Raman thermometry that we apply.Our study on first samples with a small numbers of interlayers provides not only insight into the thermal impact of each individual interface, but highlights the impact of the micropillar diameter. Building on such knowledge will allow us in future studies on larger SLs to disentangle phonon interference effects and phonon scattering phenomena.

HL 24.3 Tue 12:45 H14

Signature of thermal phonon mean free paths monitored by Raman thermometry — •Katharina Dudde[1], Mahmoud Elhajhasan[1], Guillaume Würsch[1], Julian Themann[1], Nakib Protik[2], Dwaipayan Paul[2], Giuseppe Romano[3], and Gordon Callsen[1] — [1]Institut für Festkörperphysik, Universität Bremen, Germany — [2]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [3]MIT-IMB Watson AI Lab, IBM Research, Cambridge, MA, USA

For an understanding of thermal phonon interference effects, one requires knowledge about the related phonon mean free paths l_{mfp}. In the recent past, spectroscopy methods were developed to determine l_{mfp} based on this idea: One performs thermal transport measurements under the variation of a characteristic experimental length scale L aiming to extract effective thermal properties such as the effective thermal conductivity $\kappa_{eff}(L)$. In this contribution, we analyze how non-invasive one-laser Raman thermometry (1LRT) can pose a novel option to perform thermal phonon l_{mfp} spectroscopy. Therefore, we first analyze bulk silicon at 293 K, while varying the laser focus spot radius (w_e). Here, we find a strong dependence of κ_{eff} on w_e. This dependence is more pronounced at 200 K, because l_{mfp} is increased. The second variable length scale for 1LRT is the light penetration depth (h_α), which is varied in a set of measurements for silicon membranes at 293 K. Again, a dependence of κ_{eff} on h_α is observed. Finally, our variation of w_e or h_α during 1LRT provides first insight into the impact of different thermal phonon l_{mfp} ranges on κ_{eff}.

HL 25: Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

HL 25.1 Tue 13:30 P3

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

In recent years, the emerging class of non-van der Waals 2D materials has attracted considerable interest due to the unique electronic and magnetic properties of the representatives [1]. We study here the role of spin-orbit coupling (SOC) in these non-van der Waals 2D systems and related effects that might eventually lead to topological properties. With several 2D candidates including heavy elements such as Bi and Tl, significant effects due to SOC are present in the electronic structure. For the initial screening, we employ AFLOW [2] with its standardized workflows. In a second step, we retrieve the metadata using AFLOW and adapt the extracted parameters with an AiiDA-plugin [3] for accurate electronic structure calculations using the full-potential all-electron program FLEUR [4] within AiiDA. We discuss the effect of SOC on the band structures and densities of states and also focus on the topologically protected 1D conduction edge channels [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.
[5] M. Lokamani *et al.*, manuscript in preparation (2024).

HL 25.2 Tue 13:30 P3

Influence of surface relaxations on scanning probe microscopy images of the charge density wave material $NbSe_2$ — Nikhil S. Sivakumar[1], Joost Aretz[1], •Sebastian Scherb[1], Marion van Midden Mavric[2], Nora Huijgen[1], Umut Kamber[3], Daniel Wegner[1], Alexander A. Khajetoorians[1], Malte Rösner[1], and Nadine Hauptmann[1] — [1]IMM, Radboud University, Nijmegen, The Netherlands — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, USA

Scanning tunneling microscopy (STM) images of the charge density wave (CDW) in 2H-$NbSe_2$ at voltages around the Fermi level lack a contrast inversion expected for a single-band CDW. Recent works have ascribed this to a multiband CDW or the displacement of the surface Se atoms. While STM cannot disentangle geometric and electronic structure variations, non-contact atomic force microscopy (nc-AFM) can provide better characterization of the geometric structure due to its sensitivity to the interaction between the charge densities of tip and surface. We employ distance-dependent combined constant-height STM/nc-AFM measurements to characterize the surface relaxations of 2H-$NbSe_2$. Nc-AFM images show different image contrasts depending on distance. Based on ab-initio calculations, we show that the contrast at small distances is dominated by the displacement of the surface Se atoms. For large distances, the contrast is dominated by the interaction of the permanent dipole of the tip with the potential above the surface that is predominantly modulated by the underlying Nb atoms.

HL 25.3 Tue 13:30 P3

Investigation of the electronic structure of 1T-$Ta_{1-x}Mo_xS_2$ using 11eV-laser ARPES — •Adina Timm[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The ability to modify the electronic structure of quantum materials by controlling charge density waves (CDWs) offers various possibilities for use in next-generation technologies as electronic and optoelectronic components. A material platform for testing this approach is 1T-TaS_2, which exhibits different temperature-dependent CDWs that we aim to tune by doping. Using 11eV-laser ARPES, we determine the differences in the electronic band structure of both doped and pristine TaS_2 crystals. The dopant molybdenum was introduced into TaS_2 during crystal growth by chemical vapor transport. The photoemission results show that different CDW phases are present at low doping concentrations of less than one percent with modified transition temperatures.

HL 25.4 Tue 13:30 P3

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Florian K. Diekmann[1,2], Adina Timm[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a two-dimensional hexagonal 2H structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping, making it a highly attractive candidate for spintronic applications. This assumption is supported by density functional theory calculations and scanning transmission electron microscopy studies, and RKKY interactions are predicted as the driving mechanism. The crystals investigated in this study were synthesized in-house employing the chemical vapor transport method. This process produced as-is vanadium-doped WSe_2 crystals with approximately 2% of the tungsten atoms (presumably) substituted by vanadium. The results reported here were obtained using a Physical Property Measurement System (PPMS) in ACMS configuration and provide valuable insights into the magnetic characteristics of this doped material.

HL 25.5 Tue 13:30 P3

Polarons in single-layer MoS_2 via downfolding approach to the coupling of electronic and nuclear degrees of freedom — •Laura Pätzold[1], Camiel van Efferen[2], Arne Schobert[1], Tfyeche Y. Tounsi[2], Michael Winter[1], Mark Georger[2], Afan Safeer[2], Christian Krämer[2], Jeison Fischer[2], Jan Berges[3], Thomas Michely[2], Roberto Mozara[1], Wouter Jolie[2], and Tim O. Wehling[1,4] — [1]U Hamburg — [2]U Köln — [3]U Bremen — [4]The Hamburg Centre for Ultrafast Imaging

A polaron is a quasiparticle describing a localized bound state resulting from the interaction of charge carriers with lattice vibrations. Though they are a well-studied phenomenon, experimental observations of polarons in 2D crystals are sparse. Here, we present the theoretical analysis of polaronic distortions in n-doped single-layer MoS_2 via a downfolding approach with linear electron-lattice coupling based on density functional theory calculations [1]. With this, a multi-polaronic distortion, caused by a renormalized M-point phonon, can be stabilized on supercells of up to 18×18. We compare our results to scanning tunneling microscopy measuremens obtained on n-doped single-layer MoS_2, which support the existence of polarons emerging from the coupling of non-polar zone-boundary phonons to Bloch electrons. This tunneling into the vibrationally coupled polaronic states is visible through evenly spaced peaks around the Fermi energy in the differential conductance, whose spacing matches the frequency of the M-point phonon responsible for the multi-polaronic distortion in our simulations.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

HL 25.6 Tue 13:30 P3

Electronic and phononic characterization of 2H-NbS2 at the atomic scale — •Werner M.J. van Weerdenburg, Margarete Huisinga, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDs) are a class of layered materials that can exhibit a variety of electronic properties, including low-temperature quantum phases such as superconductivity and charge density wave (CDW) formation. These phases may coexist, for instance in 2H-NbSe2, and electron-phonon interactions have been suggested as a common driving factor for the two phases [1]. In contrast, the similar compound 2H-NbS2 has a comparable superconducting critical temperature, but lacks a CDW phase [2], highlighting the importance of subtle differences in electron-phonon interactions.

Here, we apply scanning tunneling microscopy and spectroscopy (STM/STS) to investigate the electronic and phononic properties of 2H-NbS2 at the atomic scale. Based on quasiparticle interference mapping, we probe the spatial variation of the electronic density of states and identify the dispersion of the band structure around the Fermi level. Moreover, inelastic excitation spectroscopy reveals the phononic excitations of the material. By mapping the atomic-scale variation of phononic excitations around intrinsic defects of the material and adatoms, we study how electrons and phonons interact at the atomic scale.

[1] Rossnagel et al., PRB 64, 235119 (2001)
[2] Heil et al., PRL 119, 087003 (2017)

HL 25.7 Tue 13:30 P3

Characterization of surficial defect states in Mott insulator 1T-TaS_2 — •Junyoung Sim, Vibhuti Rai, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

The Mott insulating state in 1T-TaS_2, arising from strong correlations among unpaired electrons within its charge density wave superlattice, is distinct from a trivial band insulator and serves as a model system for exploring the dynamics of exotic many-body states [1]. Here, we investigate bulk 1T-TaS_2 using scanning tunneling microscopy (STM) at 5 K. We find arious nanoscopic defects including vacancies, and domain. Additionally, we adsorb transition metal adatoms on the bare surface. Using tunneling spectroscopy, we map out their electronic signatures and compare them to prior studies [2].

[1] Hellmann et al. Phys. Rev. Lett. 105, 187401 (2010)
[2] Fei et al. AAPPS Bull. 32, 20 (2022)

HL 25.8 Tue 13:30 P3

FinEstBeAMS: a multipurpose VUV and soft X-ray beamline at the max iv laboratory — •Weimin Wang, Antti Kivimäki, Kirill Chernenko, Calle Preger, and Stephan Appelfeller — MAX IV Laboratory, Lund University, PO Box 118, SE-22100 Lund, Sweden

The Finnish-Estonian Beamline for Atmospheric and Materials Science (FinEstBeAMS), located at the 1.5 GeV storage ring of the MAX IV Laboratory (Lund, Sweden), is a multidisciplinary beamline that was designed to fulfil the various needs of scientific communities in atomic, molecular and optical research, surface science, and photoluminescence research.

The gas-phase end station is equipped for electron and time-of-flight ion spectroscopies in low-density matter, while the photoluminescence end station focuses on luminescence spectroscopy of solid samples. The solid-state end station is dedicated to photoelectron and X-ray absorption spectroscopy of surfaces and interfaces, utilizing a hemispherical electron energy analyzer (PHOIBOS 150 2D-DLD from SPECS). The sample is positioned via a 5-axis motorized manipulator, offering three linear and two rotational motions (polar and azimuthal). A cryostat integrated into the manipulator enables sample cooling with liquid helium (˜50 K) and nitrogen (˜90 K). Additionally, a preparation chamber allows for sample treatment and analysis using supplementary techniques.

HL 26: Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

HL 26.1 Tue 13:30 P3

Two-dimensional hexagonal β-GeSe on Au(111) — •Dina Wilks, Veronika Blecker, Muhammad Ali Martuza, Marina Hammer, Christoph Schuster, Paulus Aleksa, and Carsten Busse — Walter-Flex-Straße 3, 57072 Siegen, Germany

Two-dimensional (2D) group-IV monochalcogenides (general form MX with M=Sn, Ge; X=S, Se, Te) demonstrate a high degree of polymorphism. While the orthorhombic phase, widely studied for its in-plane ferroelectricity, holds significant promise, experimental studies on other polymorphs remain scarce.

Here, we investigate the growth and structure of 2D hexagonal β-GeSe on Au(111). This phase is predicted to exhibit out-of-plane ferroelectricity, which could be more technologically feasible for device integration. Samples are prepared using molecular beam epitaxy (MBE) with GeSe powder as the source material and analyzed with low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). The degree of structural order was found to depend sensitively on the heat treatment. We observe a (5×5) superstructure relative to Au(111), accompanied by a continuously varying density of states (DOS) across the superstructure's unit cell. Additionally, an intriguing self-similar pattern emerges, which can be attributed to antiphase grain boundaries. These boundaries exhibit metallic behaviour near the Fermi level, highlighting their potential significance in the electronic properties of the system.

HL 26.2 Tue 13:30 P3

Scanning Tunneling Microscopy and Spectroscopy of epitaxial grown TaS_2 on GaN (0001) — •Jan-Niclas Schmidt, Constantin Hilbrunner, Georg A. Traeger, Jörg Malindretos, Angela Rizzi, and Martin Wenderoth — University of Göttingen, IV. Physikalisches Institut, Fridrich-Hund-Platz 1, 37077 Göttingen

Tantalum Disulfide crystals are interesting due to its complex phase diagram including the effect of Charge Density Waves. We are interested in how the layer thickness influences properties of Tantalum Disulfide. With Molecular Beam Epitaxy a three monolayer thick film of 2H-Tantalum Disulfide was grown on Gallium Nitride. To gain insight into the growth mechanism, the sample was transferred to a low temperature Scanning Tunneling Microscope (STM) operated at 80 K. To avoid any surface contamination, the transfer was done with a portable ultrahigh vacuum chamber. The constant-current STM-topography show small nanometer-sized, trigonal islands on a rough layer with some holes. The spectroscopy data show metallic behavior for the island as well as for the layer below.

This work is financially supported by the DFG through the SFB1073.

HL 26.3 Tue 13:30 P3

Growth dynamics of 2D materials on Ir(111) — •Smruti Ranjan Mohanty, Marko Kriegel, Frank Meyer zu Heringdorf, and Michael Horn- von Hoegen — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

The structure and morphology of 2D materials are profoundly influenced by the choice of growth substrates, with noble metal substrates offering enhanced catalytic activity and complex surface morphology facilitating precise control over the growth of 2D materials. Employing low-energy electron microscopy (LEEM), we investigated the kinetics of graphene island nucleation during the CVD of ethylene on Ir(111) at growth temperatures ranging from 750°C to 1050°C for various dosing pressures. Graphene islands nucleate heterogeneously at Ir(111) step edges, leading to edge decorations, but a transition to homogeneous nucleation occurs at island densities lower than the step density. The strong variation in island density as a function of growth temperature and dosing pressure is explained by Venables nucleation theory, with the near-linear dependence on dosing pressure attributed to a critical nucleus size (i*) of 5. The work presented here also extends to the growth and characterization of other atomically thin 2D materials, including hexagonal boron nitride (hBN), and borophene on Ir(111). The investigation reveals complex growth mechanisms, the emergence of Moiré superlattices, and substrate-influenced interactions, providing insights for designing heterostructures and functional materials with significant potential for next-generation technological applications.

HL 26.4 Tue 13:30 P3

Incommensurability and negative thermal expansion of single-layer hexagonal boron nitride — •Marko Kriegel[1], Karim Omambac[1], Steffen Franzka[2], Frank Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Carl-Benz-Str. 199, 47057 Duisburg, Germany

The emerging field of straintronics, i.e., the control and utilization of

the strain state of 2D-materials, is of great importance for their technological development, specifically in view of their future incorporation into van der Waals heterostructures. To gain fundamental insight into structural peculiarities of two-dimensional systems, single-layer hexagonal boron nitride (hBN) grown on Ir(1 1 1) by chemical vapor deposition was used as a prototypical model system: High-resolution reciprocal space mapping reveals the incommensurate nature of the material system by measuring the hBN in plane lattice parameter with high precision, facilitated by the moiré magnification effect in electron diffraction. In a growth temperature (T_g) regime of 700 to 1150°C an average lattice parameter of 2.496 ± 0.006 Å was found. Eventually, careful disentanglement of the hBN and substrate behavior for rising T_g allowed the determination of a negative thermal expansion coefficient of $\alpha_{hBN} = 2.4 \pm 1.2 \times 10^{-6}\,K^{-1}$ for free-standing hBN.[1] [1] M. Kriegel et al. Appl. Surf. Sci. 624 (2023) 157156

HL 26.5 Tue 13:30 P3

UHV-CVD on Ir(111) for the Growth of 2D Materials — •Niels Ganser[1], Marko Kriegel[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Hexagonal boron nitride (hBN) can be grown by scalable chemical vapor deposition (CVD) from a borazine $B_3N_3H_6$ precursor. Here we show that the hBN quality depends strongly on the growth temperature T_g and the dosing pressure p.

Combined SPA-LEED and LEEM measurements show a strong dependence of n on p. We find that the quality of the hBN layers that can be achieved by increasing T_g is limited by the process of disintegration of the borazine at $T_g > 950\,°C$ resulting in growth of borophene (2D Boron) instead [1]. Thus, it is possible to selectively grow either hBN or borophene from the same precursor [2].

Corroborating SPA-LEED measurements reveal a negative thermal expansion coefficient of $\alpha = (-2.4 \pm 1.2) \times 10^{-6}\,K^{-1}$ for 2D hBN in the temperature regime between 700 and 1100 °C. This finding can be explained by Lifshitz' membrane effect [3].

[1] Lifshitz, I., Zh. Eksp. Teor. Fiz. 22, 475 (1952)
[2] Omambac, K. et al., ACS Nano 15, 7421 (2021)
[3] Omambac, K. et al., ACS Nano 17, 17946 (2023)

HL 27: Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

HL 27.1 Tue 13:30 P3

Stability and electronic properties of double-layer o-B2N2 in different stacking modes — •Na Li and Claudia Draxl — Department Physics and CSMB, Humboldt-Universit at zu Berlin, D-12489 Berlin, Germany

Two-dimensional orthorhombic boron nitride (o-B2N2) has recently attracted significant attention due to its direct band gap of approximately 1.7eV and excellent visible-light absorption properties. In its layered conformations, the stacking order plays a crucial role in determining the material's stability as well as its electronic and optical properties. In this study, we employ the all-electron full potential code exciting to perform first-principles calculations of four high-symmetry bilayer stacking sequences of o-B2N2, regarding their relative stability and their electronic properties. Our calculations reveal that the AB' stacking sequence has the lowest energy and an optimized interlayer distance of 3.52 Å. The bandgaps of the AA and AA' stacking sequences are reduced relative to the monolayer, where AA' exhibits even semi-metallic behavior. In contrast, the AB and AB' stacking sequences show slightly increased direct bandgaps.

HL 27.2 Tue 13:30 P3

In-depth analysis of stratified MoS2 and WS2 2D heterostructures — •Sebastian Klenk, Nikolas Dominik, Cormac Ó Coileáin, Tanja Stimpel-Lindner, and Georg S. Duesberg — University of the Bundeswehr Munich, Institute of Physics, Germany

Starting with graphene roughly two decades ago, two-dimensional (2D) materials have garnered great interest in the scientific community due to their exceptional electrical, mechanical and optical properties. The broad palette of different 2D materials has allowed for the possibility to change and finetune these parameters to one's own liking by combining several 2D materials in one film. Here, we present the metal-organic chemical vapour deposition (MOCVD) synthesis and analysis of MoS2/WS2 heterostructures. We show the ordering of a high-quality 7-layer combination structure of less than 10 nm. The layered nature is confirmed and discussed using XPS, EDX, ToF-SIMS, TEM, AFM and Raman spectroscopy.

HL 27.3 Tue 13:30 P3

A Two-dimensional Heterostructure Fabrication System in Ultra-high Vacuum — •Daiyu Geng, Jiabao Yang, Natalie Lehmann, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

We develop an ultra-high vacuum system for the fabrication of two-dimensional heterostructures. The clean transfer and stacking of two dimensional material flakes are realized using a polymer-free method based on SiNx cantilevers coated with Au film (Nature Electronics, 2023, 6(12): 981-990). The system also incorporates multiple surface preparation and characterization techniques like MBE, Plasma sputtering and electron diffraction. All these methods enable us to prepare heterostructures with atomically clean interface, which is important for the spectroscopic investigation of the rich physics effects in two-dimensional heterosystems.

HL 27.4 Tue 13:30 P3

Exploring MXenes as Electrodes for Al-ion Batteries: An Ab-initio Study on the Impact of Stacking Configurations and Termination Types — •Amal Raj Veluthedath Nair and Nuala M Caffrey — School of Physics, University College Dublin, Dublin 4, Ireland

MXenes, with their tunable surface chemistry, thin 2D structures, large interlayer spacing, and good conductivity, are promising candidates for battery electrodes. The stacking configuration of MXene layers, determined by their chemistry and surface terminations, influences their electrochemical performance.

This study explores Ti_3C_2 and V_2C MXenes as electrodes for Na, Mg, and Al-ion batteries using density functional theory. We examine four stacking configurations and two coordination sites for intercalated ions. Results reveal that stacking configuration and surface terminations significantly influence change in interlayer distance, with O-terminated octahedral stacking showing the least change in spacing for all intercalants. The smallest interlayer distance change occurs for Al intercalation in V_2C, with a Δd of 0.1 Å, matching experimental findings (Vahidmohammadi et al., 2017). Ion migration studies indicate that prismatic stacking promotes faster ion migration compared to octahedral stacking. O-terminated MXenes significantly enhance the theoretical specific capacity for Al intercalation, reaching a maximum value of 283.48(277.63)mAh/g for $Ti_3C_2O_2(V_2CO_2)$. In contrast, F-terminated MXenes show much lower capacities.

HL 27.5 Tue 13:30 P3

Triplet pairing enabled proximity superconductivity in monolayer WTe_2 — •A. Bäder[1,2], T. Wichmann[1,3], J. Martinez-Castro[1,4], P. Rüssmann[5,6], K. Jin[1,4], T. Samuely[7], Z. Lyu[1,3], J. Yan[8], O. Onufriienko[7], P. Szabó[7], F. S. Tautz[1,3], M. Ternes[1,4], S. Lounis[5,9], and F. Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Experimentalphysik IV A, RWTH Aachen — [4]Institut für Experimentalphysik II B, RWTH Aachen — [5]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich — [6]Julius-Maximilians-Universität Würzburg, Fakultät für Physik und Astronomie — [7]Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University & Institute of Experimental Physics, Slovak Academy of Sciences — [8]Materials Science and Technology Division, Oak Ridge National Laboratory, USA — [9]Fakultät für Physik, Universität zu Duisburg-Essen

We use low-temperature scanning tunneling microscopy to investigate proximity-induced triplet pairing and its role in enabling supercon-

ductivity in a monolayer $WTe_2/NbSe_2$ van der Waals heterostructure. Employing the Kohn-Sham Bogoliubov-de Gennes formalism, we find that conventional s-wave pairing fails to induce superconductivity in the WTe_2, in contrast to triplet pairing. Applying an external magnetic field, we examine Abrikosov flux vortices within the heterostructure and exploit them to probe local superconducting properties. Our findings highlight a platform for studying triplet pairing-induced superconductivity with potential topological characteristics.

HL 28: Topological Insulators (joint session MA/HL)

Time: Tuesday 14:00–15:15 Location: H16

HL 28.1 Tue 14:00 H16

Topological Hall effects on two-dimensional Archimedean lattices — •L.V. Duc Pham[1,2], Nicki F. Hinsche[2], and Ingrid Mertig[2] — [1]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, Bergstraße 66c, 01062 Dresden, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany

Archimedean lattices are a family of tilings in which the two-dimensional plane is filled with different regular polygons while maintaining the vertices configuration. Kagome, the most famous member of the Archimedean lattices familiy, was studied extensively in a wide variety of theoretical works. Another lattice of this type, the snub square lattice, was also used as an approximant for quasi crystals [1]. The rich geometry of these systems gives rise to various unconventional nano ribbon edge configurations and therewith various possible topological edge states. In this work, we calculate the band structures of all 8 pure Archimedean lattices using a tight-binding method including s and p orbitals and study topological properties of these lattices, such as topological edge states, the $\mathbb{Z}_2$ invariance and the quantum spin Hall conductivity within the Kubo formalism [2].

[1] Roy, Sumalay, et al. "The Kepler tiling as the oldest complex surface structure in history: X-ray structure analysis of a two-dimensional oxide quasicrystal approximant." Zeitschrift für Kristallographie-Crystalline Materials 231.12 (2016): 749-755

[2] Sinova, Jairo, et al. "Spin hall effects." Reviews of modern physics 87.4 (2015): 1213-1260

HL 28.2 Tue 14:15 H16

Spin topology, spin-orbit coupling and entanglement — •Gunnar Felix Lange[1], Wojciech Jankowski[2] und Robert-Jan Slager[2,3] — [1]Department of Physics, University of Oslo, Norway — [2]TCM Group, Cavendish Laboratory, University of Cambridge, UK — [3]Theoretical Physics Group, University of Manchester, UK

Topological systems with time-reversal symmetry are of great theoretical and practical interest. Theoretically, such phases often rely on studying the topology in each spin sector separately, as in the spin Hall effect.

This requires identifying the spin degree of freedom in the band structure, which is not always straightforward in the presence of spin-orbit coupling. This field has received renewed interest in recent years, leading to the concept of spin topology.

In this talk, we will discuss some recent results on spin topological phases, with a particular focus on spin-orbit coupling and its interplay with entanglement.

HL 28.3 Tue 14:30 H16

Fractionally Charged Vortices at Quantum Hall/Superconductor Interfaces — •Enderalp Yakaboylu and Thomas Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg

We investigate interface states between a type-II s-wave superconductor (SC) and a Chern insulator describing an integer quantum Hall (QH) system. We find that an effective pairing interaction at this boundary gives rise to two emergent Abelian Higgs fields, representing the two paired electrons at the SC/QH interface, coupled to a gauge field that incorporates both Chern-Simons and Maxwell terms. We use this model to investigate the effect of magnetic flux vortices in the SC on the QH system. In particular, we find vortex solutions in which the Cooper pairs give rise to topological fractionally-charged vortices localized at the interface.

HL 28.4 Tue 14:45 H16

Local and Global Topological Characteristics of Local Magnetic Moments Coupled to Chern Insulators — •Devesh Vaish and Michael Potthoff — I. Institute of Theoretical Physics, Department of Physics, University of Hamburg

A magnetic impurity, modelled as a classical spin and locally exchange coupled to a Chern insulator may cause in-gap bound states. Their nature can be very different depending on the (k-space) topological phase of the Chern insulator. Here we study several impurity spins coupled to a QWZ model and analyze, for different k-space topological phases, the additional "local" topological properties on the manifold of impurity-spin configurations (S-space). In case of $R > 1$ spins, the R-th spin-Chern number serves as a topological invariant on S-space. Varying the local exchange-coupling strength, we find local topological phase transitions and relate them to Fermi-energy crossings of in-gap states. In addition, we compute the first spin-Chern number for various physically motivated closed two-dimensional sub-manifolds of the full configuration space and relate those to the R-th spin-Chern number.

HL 28.5 Tue 15:00 H16

Non-relativistic linear Edelstein effect in noncollinear EuIn2As2 — •Adriana Nayra Alvarez Pari[1], Rodrigo Jaeschke Ubiergo[1], Atasi Chakraborty[1], Jairo Sinova[1,5], and Libor Smejkal[1,2,3,4] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany — [2]Max Plank Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic — [5]Department of Physics, Texas A & M University, Texas, USA

Motivated by the ongoing interest in understanding the actual magnetic ground state of the promising axion insulator candidate EuIn2As2, we present here a spin symmetry analysis and *ab-initio* calculations, aiming to identify specific exchange-dominated physics that could offer insights into the current debate. We investigate two non-collinear coplanar magnetic orders reported in this compound: the *helical* and *broken-helical* phases [1]. Our symmetry analysis shows that magnetic-exchange alone results in the formation of an out-of-plane odd-wave order in momentum space in both phases. Additionally, we identify an in-plane g-wave order that emerges exclusively in the *broken-helical* phase, providing a distinguishing feature for this phase. Furthermore, we report a non-relativistic Edelstein effect with a distinct out-of-plane polarized spin density that dominates over spin-orbit coupling effects.

[1] Pari, Nayra A. Álvarez, et al. "Non-relativistic linear Edelstein effect in non-collinear EuIn2As2." *arXiv:2412.10984* (2024)

HL 29: Poster II

The second poster session on the physics of semiconductors covers topics from 2D semiconductors and van der Waals heterostructures, the physics of the van der Waals magnetic semiconductor CrSBr, materials and devices for quantum technology, quantum dots and wires, transport properties, to ultrafast phenomena in semiconductors.

Time: Tuesday 18:00–20:00 Location: P1

HL 29.1 Tue 18:00 P1

Electrical Field Effect and Schottky Barriers in $FePSe_3$ Thin Films — •Paul Perl[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Transition metal selenophosphates (MTPs) are a group of promising 2D materials for applications like transistors and photodetectors [1,2]. Among MTPs, iron selenophosphate ($FePSe_3$) has one of the lowest band gap energies at 1.3 eV [2]. The goal of this work is to examine the influence of the electric field effect on electrical transport and to study the Schottky barriers formed at metal contacts. Moreover, the temperature dependence of the investigated effects is analyzed.

In order to investigate the electrical properties of $FePSe_3$ in thin films below 30 nm, layers are mechanically exfoliated onto a Si/SiO_2 substrate. Electrical contacts for the exfoliated flakes are fabricated via electron beam lithography and physical vapor deposition. $FePSe_3$ exhibits a hysteresis in its transport characteristics when the applied backgate voltage is altered, indicating favorable characteristics for memory devices. Furthermore, differences in Schottky barriers for various contact material compositions become apparent, showing their influence on electric transport properties.

[1] T. Xu et al., Advanced Electronic Materials, 7, 2100207 (2021)
[2] M. A. Susner et al., Advanced Materials, 29, 1602852 (2017)

HL 29.2 Tue 18:00 P1

Fabricating MoS_2 nanotube quantum dots on 2D heterostructures — •Korbinian Fink[1], Robin T. K. Schock[1], Stefan B. Obloh[1], Matthias Kronseder[1], Matjaž Malok[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg — [2]Solid State Physics Department, Jožef Stefan Institute, Ljubljana, Slovenia

MoS_2, a transitional metal dichalcogenide (TMDC) with interesting optical and electronic properties, e.g., broken inversion symmetry and strong spin-orbit coupling leading to spin split bands, is at the center of manifold research efforts. Building a MoS_2 based QD remains challenging: the spatial quantization depends on the effective electron mass, which is high in MoS_2, and minuscule devices sizes are required.

In order to reduce the lithographic constraints we utilize nanotubes, as these confine charges in an additional dimension. However, these QDs are still limited by the disorder from the SiO_2 surface. This can be resolved by fabricating the devices on top of 2D heterostacks consisting of hBN and few layer graphite.[1]

The major challenge for creating such devices is reproducible contacts to the nanotubes, as nanogaps between the contact on the chip and the metal on top of the tube lead to high resistance variations. This can be solved by variation of the incident angle and heating during metalisation as well as fixing the tubes on the chip by cross linked resist. - [1] R. T. K. Schock et al., PSSb, 2400366 (2024)

HL 29.3 Tue 18:00 P1

Preparation of folded graphene heterostructures via dry transfer — •Hannes Kakuschke[1], Dustin Wittbrodt[2], Lina Bockhorn[1], and Rolf Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Mono- and bilayer systems of graphene have been extensively researched due to their unique magnetic and electronic transport properties. In more recent work, folded graphene [1, 2] heterostructures exhibit fascinating phenomena. This is due to the topology of the folded region, causing effects such as snake states and zero line modes. However, in transport measurements of self-assembled, folded graphene [3], multiple effects occur simultaneously. This drastically complicates the analysis of individual contributions. To solve this problem, we use the dry transfer method to fold graphene around hBN, decoupling the overlapping graphene regions.

To simulate the behaviour of such samples, Tight-Binding model calculations [4], considering strain effects [5] at the folded edge have been carried out.

[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).
[4] M. Koshino & T. Ando, Solid State Commun. 149, 1123-1127 (2009).
[5] A. R. Botello-Méndez et al., JPC C. 122 (27), 15753-15760 (2018).

HL 29.4 Tue 18:00 P1

Ferroelectric Potential Investigations of 3R MoS_2 through fast Optical Measurements — •Jan-Niklas Heidkamp[1], Swarup Deb[1,2], Takashi Taniguchi[3], Kenji Watanabe[3], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]National Institute for Material Science, Tsukuba, Japan

In recent years, sliding ferroelectricity has emerged as a topic of significant interest due to its possible application in nonvolatile random-access memory. This phenomenon is unique to two-dimensional van der Waals materials, where vertical polarization switching is induced by in-plane sliding of the constituent layers. The resulting polarization is influenced by the intrinsic stacking order, creating distinct polarization regions separated by domain walls. These regions, along with the domain walls, can be manipulated using an external vertical electric field, enabling a switchable system that retains the environmental robustness of van der Waals materials under ambient conditions.
In this study, we investigate 3R-MoS_2 using various optical measurement techniques at room temperature. The spatially resolved measurements reveal clear signal changes corresponding to different ferroelectric stacking orders and variations in layer count. Our findings demonstrate that fast optical mapping at room temperature is a reliable method for probing ferroelectric potential steps in 3R-stacked samples. This approach does not require a conductive substrate or backing, making it more versatile than traditional Kelvin Probe Force Microscopy (KPFM) techniques.

HL 29.5 Tue 18:00 P1

Probing TMD-nanowire hybrid structures with second harmonic generation. — •Benedikt Mathes, Maximilian Tomoscheit, Edwin Eobaldt, Alexander Zaunick, Carsten Ronning, and Giancarlo Soavi — Institut of Solid State Physics, University of Jena

Hybrid nanostructures have been drawing attention in fundamental science, since they allow to control and engineer the electronic and optical properties of samples. Transition metal dichalcogenide(TMD)-nanowire(NW) hybrid structures could have interesting applications beyond fundamental science, since they allow to tune the lasing properties of NW lasers. To understand the photo-physical response of the hybrid system, it is helpful to measure the optical and electronic response of each of its individual constituent. However, this is in general difficult to achieve. In this work, we solve this problem by showing that polarization-dependent second harmonic generation(SHG) can selectively probe each constituent of a WSe_2-ZnO NW hybrid, provided that the subsystems are properly and deterministically aligned. TMDs exhibit a threefold symmetry with two main axes, armchair(AC) and zigzag(ZZ). When excited along the ZZ axis, the SH is emitted along the AC axis, whereas the SH of the NW is always emitted parallel to its long axis. Hence, by aligning the NW along the ZZ axis one can differentiate the emission from NW and TMD with a polarizer in detection aligned along the ZZ or AC axis, respectively. This way, the subsystems of the hybrid structure can be investigated individually, offering new insights into their contribution to the hybrid system.

HL 29.6 Tue 18:00 P1

Raman and photoluminescence spectroscopy on differently

synthesised $MoSe_2$ — •Lara Blinov[1], Hendrik Lambers[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

There are various synthesis methods for the widely researched transition metal dichalcogenides (TMDCs). We examine optical responses of $MoSe_2$ synthesised by chemical vapor transport (CVT) with different halogen contributions in the transport gas. Therefore, mono- and bilayers of those differently grown parental crystals are mechanically exfoliated and investigated by Raman and photoluminescence (PL) spectroscopy at room temperature as well as in temperature-dependent PL measurements.

We analyse and compare the energies and intensities corresponding to the neutral A and B excitons as well as a prominent A^- trion in the PL spectra and the frequency of the first order Raman modes. We conclude that the CVT synthesised crystals seem to have an inhomogeneous distribution of charge carrier densities or defects and that the defect density seems to be larger than in conventionally synthesised $MoSe_2$.

HL 29.7 Tue 18:00 P1

Optical Properties of Janus Transition Metal Dichalcogenides — •Sai Shradha[1], Julian Picker[2], Nicole Engel[1], Lukas Krelle[1], Daria Markina[1], Roberto Rosati[3], Ermin Malic[3], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Institute for Physical Chemistry, Friedrich Schiller University, Jena, Germany — [3]Department of Physics, Philipps-Universität Marburg, Marburg, Germany

Janus transition metal dichalcogenides (JTMDs) have a crystal structure of X-M-Y where X and Y are chalcogens and M is a transition metal. Their asymmetric structure, with chalcogen atoms of different electronegativity above and below the transition metal, leads to an intrinsic out-of-plane electric dipole. This out-of-plane symmetry breaking in JTMDs causes Rashba splitting, vertical piezoelectricity and enhanced exciton-phonon coupling. Due to a reduced overlap of the electron and hole wave functions, excitons in JTMDs are predicted to have lower binding energies and longer lifetimes. This makes them promising candidates for photovoltaic devices. Via chemical vapour deposition (CVD), high-quality Janus monolayers have been synthesised [1]. This work investigates the optical properties of CVD-grown monolayer Janus MoSSe and WSSe. Photoluminescence, Raman and differential reflectivity spectroscopy performed at room temperature and 4K are used as the key techniques to identify and further analyse excitons and exciton-phonon coupling in such systems.

[1] Z. Gan et. al., Adv. Mater., 34, 2205226 (2022)

HL 29.8 Tue 18:00 P1

Microscopic, Optical, and Electrical Characterization of Spray-Coated Graphene Dispersions on Sapphire Substrates — •Yasaman Jarrahi Zadeh[1], Lars Grebener[2], Muhammad Ali[3], Felix Schaumburg[1], Mohaned Hammad[2], Günther Prinz[1], Martin Geller[1], Hartmut Wiggers[3], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics, and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Energy and Materials Processes, and CENIDE, University of Duisburg-Essen, Germany — [3]Institute for Combustion and Gas Dynamics, and CENIDE, University of Duisburg-Essen, Germany

Processing graphene into thin films is crucial for its potential in cutting-edge applications. Here, we report on different characterization techniques to analyze the dispersion and coating performance of spray-coated graphene films on sapphire substrates. The deposited films were characterized using optical and scanning electron microscopy to evaluate coating morphology. Raman Spectroscopy and electrical characterization were used to assess the structural integrity and functional performance of the constituent graphene sheets. The deposited films fabricated from graphene sheets dispersed in water with carboxymethyl cellulose (CMC) exhibited uniform surface morphology compared to deposition with ethanol dispersion. Raman spectroscopy and electrical characterization confirmed the quality and structural integrity of the water-CMC dispersion. This study highlights key process-structure relationships for optimizing dry-synthesized graphene films for advanced technologies.

HL 29.9 Tue 18:00 P1

Vibrational fingerprint of 2D transition-metal dichalcogenide WSe_2 — •Kanivar Türk, Bastian Thomssen, Gerhard Berth, and Klaus Jöns — PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany

Thin-layered transition-metal dichalcogenides (TMDC) are on high demand in the material science community [1]. The advantages of monolayer configurations of these TMDCs include the transition from indirect to direct band gap, which leads to way superior properties when compared to bulk, like optical, electrical, magnetic, thermal and mechanical improvements [2].
In this work, exfoliated 2D flakes of WSe_2 have been produced and analysed in terms of their vibrational properties via Raman spectroscopy. Beside a comprehensive phonon mode assignment, a layer number specific analysis has been performed and compared to results from photoluminescence measurements.

[1] Saju Joseph et al.; Materials Chemistry and Physics 297: A review of the synthesis, properties, and applications of 2D transition metal dichalcogenides and their heterostructures (2023)

[2] Mingxiao Ye et al.; Photonics, 2: Recent Advancement on the Optical Properties of Two-Dimensional Molybdenum Disulfide (MoS_2) Thin Films (2015)

HL 29.10 Tue 18:00 P1

Tuning of excitonic emission of 2D-TMDs by hybridization with phase change materials — •Jakob Cornelius Wurschi, Martin Hafermann, Edwin Eobaldt, and Carsten Ronning — Institut für Festkörperphysik FSU Jena

Transition metal dichalcogenides (TMDs) are a subject of growing interest, given their wide range of potential applications, such as transistors or biosensors. Especially in the context of optoelectronic devices a precise tuning of the emission behaviour can be a powerful tool for the realisation of advanced technologies. To gain insight into potential tuning mechanisms of the excitonic emission of TMD monolayers, we investigate the hybridization of 2D MoS_2 and WS_2 flakes with germanium-antimony-telluride (GST). This compound system is capable of undergoing a phase transition between an amorphous and two crystalline states accompanied with drastic changes in the electrical and optical properties. Thermal heating triggers the phase transitions of GST, which we monitor by measuring the reflectivity of the GST thin films on silicon. After 2D-TMD flake exfoliation, in-situ measurements of the TMD photoluminescence spectra were obtained during or after the phase transitions of the GST substrate. With our approach, we observe a significant spectral shift of the excitonic emission of MoS_2 on GST/Si by precisely tuning the phase of the underlying GST. Further, for WS_2 flakes on gold substrates we observed a GST layer thickness dependent spectral shift for the excitonic emission of WS_2.

HL 29.11 Tue 18:00 P1

Gate defined exciton confinement in $MoSe^2$. — •Moritz Scharfstädt[1], Abdul R. Kanikode[1], Lasse Ebeling[2], Max Wegerhoff[1], Michael Köhl[1], Stefan Linden[1], Bernd Beschoten[2], Christoph Stampfer[2], Lutz Waldecker[2], and Andrea Bergschneider[1] — [1]Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany — [2]II. Physikalisches Institut, RWTH Aachen University, 52074 Aachen, Germany

Excitons in transition metal dichalcogenides (TMDs) are ideal candidates for strong light-matter interactions due to their high oscillator strength. This has been demonstrated in numerous experiments where 2D semiconductors were embedded in photonic cavities. However, these systems lack strong nonlinearity, necessitating further efforts to realize applications such as single-photon sources. One possible approach could be the spacial confinement of excitons using an in-plane inhomogeneous electric field, as first demonstrated by [1].

We present measurements on a similar system that achieves 1D confinement of excitons along the edge of a few-layer graphene gate. While the excitons are polarized perpendicular to the edge, we observe two orthogonal linear polarization axes of the confined states. This raises questions about the selection rules in such a system.

Furthermore, we show our approach to shape the confinement into a 0D configuration to enhance exciton-exciton interactions and, presumably, the system's nonlinearity.

HL 29.12 Tue 18:00 P1

PROBING INTERLAYER EXCITONS IN PARALLEL STACKED FERROELECTRIC MOS2 — •Johannes Krause[1],

Jan-Niklas Heidkamp[1], Swarup Deb[3], Kenji Watanabe[2], Takashi Taniguchi[2], Rico Schwartz[1], and Tobias Korn[1] — [1]University of Rostock, Insitute of Physics, Germany — [2]International Center for Materials Nanoarchitectonics, National Institute for MAterials Science, Tsukuba — [3]Saha Institute of Nuclear Physics, Kolkata, India

2D Transtion Metal Dichalcogenides (TMDCs) garnered significant scientific interest, due to their unique optical properties. Interestingly, 3R-stacked TMDCs exhibit sliding ferroelectricity, which opens up new platforms for nanoelectronic and memory devices. Here, we investigate the photoluminescene (PL) associated with a 3R-stacked molybdenum disulfide homobilayer, particularly the signals attributed to the interlayer exciton. Additionally, electric fields are applied to control the characteristic properties of the stack. We employ mechanical exfoliation of bulk 3R-grown MoS2-crystals and the deterministic transfer technique to fabricate and transfer the homobilayers onto SiO2 wafers with pre-patterned electrical contacts. We utilize PL measurements to characterize the relevant optical signals. By applying gate voltages across the homobilayer, we explore the optical behavior of the homobilayer stack, enabling precise modulation of exciton properties by controlling charge carrier density and Stark effect.

HL 29.13 Tue 18:00 P1

Moiré superlattice effects in $MoSe_2$-WS_2 heterobilayers — •P. Parzefall[1], N. Paulik[1], M. Lorenz[1], C. Serati de Brito[1,2], J. Göser[3], J. Trapp[3], T. Taniguchi[4], K. Watanabe[4], A. Högele[3], Y. Galvão Gobato[2], and C. Schüller[1] — [1]Institut für Exp. und Angewandte Physik, Uni Regensburg (UR), Germany — [2]Physics Department, Federal University of São Carlos, Brazil — [3]Faculty of Physics, Munich Quantum Center and Center for NanoScience, LMU Munich, Germany — [4]NIMS, Tsukuba Ibaraki, Japan

We report about optical studies on type-I $MoSe_2$-WS_2 heterostructures at cryogenic temperatures. We confirm the influence of the moiré superlattice on excitonic features of angle aligned R- and H-type structures in photoluminescence spectroscopy. The moiré-exciton and moiré-trion features are further studied by resonant low-frequency Raman spectroscopy. Here, we tune a Ti:Sapphire laser into close resonance to the $MoSe_2$ intralayer excitonic transitions. We detect an efficient pumping of the moiré trion when exciting resonantly to the moiré exciton, as the binding energy is equivalent to a phonon energy.

In time-resolved measurements using a Streak camera, we measure the lifetimes of both H-type and R-type moiré-excitonic species. The detected short excitonic lifetimes in the R-type sample is indicative of a type-I band alignment and the longer moiré-exciton lifetimes in the H-type samples might be due to a hybridization in the conduction bands [1, 2]. [1] B. Polovnikov et al., Phys. Rev. Lett. 132, 076902 (2024), [2] Y. Galãvo Gobato et al., Nano Lett. 22, 8641 (2022)

HL 29.14 Tue 18:00 P1

Acousto-optic characterization of van der Waals systems — •Felix Ehring, Benjamin Mayer, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

With wavelengths in the micrometer range at GHz frequencies, surface acoustic waves (SAWs) are a versatile tool for radio frequency control and probing of charge carrier dynamics in novel semiconductor nanostructures. They are generated on a piezoelectric chip and routed over long distances to couple either mechanically or electrically with almost any nanosystem [1]. In our experiments, we fabricated hybrid lithium niobate SAW-devices including SAW delay lines with design frequencies of 150-250MHz, on which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials can be placed. The dynamic strain and electric field of the SAW induce a band modulation in the TMDC structure. The focus of the experiments was the investigation of MoSe2-WSe2 heterostructures and their interlayer excitons. For the characterization, the influence of the SAW fields on the recombination time and energy was investigated. Since interlayer excitons provide a much longer lifetime than intralayer excitons, transport along the propagation direction of the wave should be possible and will be part of future experiments. [1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 29.15 Tue 18:00 P1

Influence of interface dielectric disorder on interlayer excitons in mixed binary/ternary TMD heterostructures — •Mohammed Adel Aly[1,2], Emmanuel Oghenevo Enakerakpor[2], Hilary Masenda[2], and Martin Koch[2] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [2]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

The unique properties of transition metal dichalcogenide (TMD) monolayers and their heterostructures offer exceptional tunability. In these heterostructures, interlayer excitonic emission can be tailored based on the selection of the monolayer materials. In this study, we fabricated heterostructures based on binary-ternary monolayers, which offer enhanced tunability of the interlayer exciton emission. To understand the physics behind the interlayer excitons and their photoluminescence linewidths, we measured the photoluminescence of excitons in two TMD heterostructures, MoSe2/Mo0.5W0.5Se2 and WSe2/Mo0.5W0.5Se2, at different temperatures ranging from 10 K - 300 K. Besides neutral excitons and trions, we found that the linewidths of interlayer excitons are significantly broadened due to dielectric disorder caused by the spatial inhomogeneity at the interfaces of the heterostructures. These are important for our understanding of the nature of the interlayer excitons and their tunability for future optoelectronic devices.

HL 29.16 Tue 18:00 P1

High-Pressure Optical Spectroscopy of Intralayer and Interlayer Excitons in 2H-MoS_2 Bilayers — •Vedhanth Senthiappan Vellaiappan Uthayasurian, Paul Steeger, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Molybdenum disulfide (MoS_2) is a van der Waals material from the class of Transition Metal Dichalcogenides (TMDCs). In 2H-MoS_2 homo-bilayers, interlayer excitons, where the electron and hole are located in different layers, are observed with a large oscillator strength and distinct energy separation from intralayer excitons. We investigate these inter- and intralayer excitons in 2H-MoS_2 homo-bilayers under applied pressure using a diamond anvil cell [1]. Optical transmission spectra reveal that increasing pressure reduces the energy splitting between the A exciton and the interlayer exciton. Ab initio calculations, combined with our experimental observations, indicate that this behavior cannot be attributed to conventional hydrostatic compression. Instead, it results from the MoS_2 bilayer adhering to the diamond surface, which limits in-plane compression. Furthermore, we show that the unique real-space distributions and the associated contributions from the valence band are responsible for the differing pressure responses of the inter- and intralayer excitons in compressed MoS_2 bilayers. References : [1] P. Steeger et al, Nano Lett., 23, 8947 (2023)

HL 29.17 Tue 18:00 P1

Magneto-Optical Spectroscopy of van der Waals CrSBr — •Lukas Krelle[1], Ryan Tan Qai Shen[1], Daria Markina[1], Priyanka Mondal[1], Kseniia Mosina[2], Kevin Hagmann[1], Regine von Klitzing[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

The layered antiferromagnet CrSBr is a promising Van der Waals material due to its quasi 1D nature and the strong coupling between excitons, phonons and magnons. In particular, the strong coupling of excitons to the magnetic order of the crystal opens new avenues for the study of correlated magnetic phases in optical spectroscopy. In this work, we perform magneto-optical spectroscopy on multilayer CrSBr. We use Photoluminescence and Reflectivity measurements to identify the different magnetic phases present in the sample. We report drastic changes of the emission and absorption depending on the magnetic phase of the material, which we control through the application of magnetic fields along specific directions.

HL 29.18 Tue 18:00 P1

Raman investigation of the 2D magnetic semiconductor $MnPS_3$ — •Thomas Kliewer[1], Pierre-Maurice Piel[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

The van-der-Waals (vdW) material $MnPS_3$ is a member of the group of metal phosphorus trichalcogenides (MPX_3; X=S, Se) which experiences rising interest due to its rich physical, chemical and structural properties. $MnPS_3$ is a 2D magnetic semiconductor with an electronic

bandgap of 2,79 eV[1]. Below the Néel-Temperature of 78 K, it exhibits an antiferromagnetic order within the layers and a ferromagnetic coupling between adjacent layers[2]. These properties are interesting for fundamental studies on magnetism in the 2D limit, the investigation of coupling between spin, lattice and charge degrees of freedom and for possible applications in spintronics. $MnPS_3$ flakes of various thicknesses have been studied by temperature dependent Raman spectroscopy to uncover the coupling of lattice and spin degree of freedom. The Raman-spectra of $MnPS_3$ show several phonon modes in accordance with the crystal structure. The intensity of the modes varies with the thickness of the crystal. Besides the expected hardening of the modes, the temperature-dependent measurements imply possible influence of the magnetic ordering on the observed modes. [1] Grasso et al. Physical Review B 44.20 (1991), p. 11060 [2] Wildes et al. Journal of Physics: Condensed Matter 6.24 (1994), p. L335

HL 29.19 Tue 18:00 P1

Polarisation dependant reflectance measurements of CrSBr — •Manuel Terbeck, Aleksandra Lopion, Pierre-Maurice Piel, and Ursula Wurstbauer — Institute of Physics, University of Muenster, Germany

The van der Waals layered material CrSBr has multiple interesting characteristics. It is an air-stable, optically active magnetic semiconductor. Magnetically, CrSBr exhibits ferromagnetic ordering in-plane and antiferromagnetic ordering between adjacent layers, with the easy axis being in-plane [1]. In this material the coupling between magnetic and optical properties is strong allowing us to study magnetic properties by measuring interband emissions and absorption spectra. The electronic structure is often described as quasi-1D due to the highly anisotropic properties [1]. Thus the polarisation of light is important when measuring CrSBr optically. With Raman scattering, we checked the symmetry of the crystal. Considering those axes, we measured reflectance from thin CrSBr flakes using different polarisation of light to get information about the excitonic states in this material. Unlike emission, reflectance measurements enables additional access to higher electronic states. [1] J. Klein, et al. ACS Nano, 17, 5316-5328 (2023)

HL 29.20 Tue 18:00 P1

Semiconductor-Metal Interfaces in 2D TMDCs for High-Efficiency Optoelectronic Devices — •Linus Schneider[1], Ariane Ufer[1], Elena Vinnemeier[1], Rebecca Saive[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]MESA+ Institute for Nanotechnology University of Twente, Enschede, Netherlands

Efficient solar energy conversion requires new materials and technologies that enhance solar cell performance while minimizing material usage. Two-dimensional (2D) materials, specifically transition metal dichalcogenides (TMDCs) like molybdenum disulfide (MoS_2), exhibit strong exciton-mediated light-matter interactions, making them ideal for optoelectronic devices and solar energy conversion. A critical challenge for implementation is effective charge carrier extraction at the metal-semiconductor interface. We prepare TMDC flakes using mechanical exfoliation and fabricate semiconductor-metal junctions by transferring these layers onto metallic contacts using a dry viscoelastic stamping technique. The structural and optical properties of these samples are characterized using photoluminescence (PL) and Raman spectroscopy. The charge transfer behavior at the 2D semiconductor-metal interface is probed by localized laser beam-induced current measurements and the local potential change across the junction regions by kelvin probe force microscopy (KPFM).

HL 29.21 Tue 18:00 P1

Advancing 2D Materials for Optoelectronic and Photonic Devices: Insights from WSe_2 — •Bastian Thomssen, Ioannis Caltzidis, and Klaus D. Jöns — PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany

Two-dimensional (2D) materials have garnered significant attention due to their unique structural, electronic, and optical properties, which make them ideal candidates for next-generation optoelectronic and photonic devices. [1] Transition metal dichalcogenides (TMDs), such as tungsten diselenide (WSe_2), exhibit remarkable characteristics: in monolayer form, WSe_2 transitions from an indirect to a direct bandgap semiconductor, enhancing light-matter interactions. This property positions WSe_2 as a promising material for applications in light-emitting diodes, lasers, and quantum emitters. [1] The layer-dependent properties of WSe_2, including the transition from an indirect to a direct bandgap, can be effectively characterized using photoluminescence measurements. These allow for precise determination of the layer number, providing valuable insights into the electronic and optical behavior of the material. Such measurements are essential for tailoring the material's properties for specific optoelectronic and photonic applications.

[1] Maja Groll et al. https://doi.org/10.1002/smll.202311635

HL 29.22 Tue 18:00 P1

Having a Good Vibe: Electron-Phonon Coupling in 1L-TMDCs Measured by Transient Absorption Spectroscopy — Tim Völzer[1,2], •Julian Schröer[1,2], Marvin Krupp[1,2], Annika Bergmann[1,2], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]University of Rostock, Institute of Physics — [2]Department "Life, Light & Matter, University of Rostock

The optoelectronic properties of monolayer transition metal dichalcogenides (1L-TMDCs) are strongly determined by their electronic dynamics after light excitation. In this work, we present insights on the ultrafast dynamics of three different 1L-TMDCs by employing transient absorption (TA) spectroscopy. Our findings show that the basic processes after optical excitation can be divided into cooling of the electronic and phononic system and the subsequent recombination of the excited species. We reveal the importance of the differing coupling strengths to high- versus low-energy phonons. Due to the ultrashort pump pulse excitation, we are also able to trigger the displacive excitation of coherent phonons, which we assign to the A'_1 Raman mode of the system. Our results demonstrate the strong coupling between the electronic and phononic systems and lead to better understanding of excited state carrier dynamics in 1L-TMDC materials.

HL 29.23 Tue 18:00 P1

Probing time-reversal symmetry breaking in graphene — •Konrad Krieghoff[1], Nele Tornow[1], Omid Ghaebi[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

In graphene, space inversion symmetry (SIS) and time-reversal symmetry (TRS) combined with a hexagonal lattice give rise to a linear band dispersion at the +/−K points of the Brillouin zone. Breaking TRS can result in exotic phenomena, such as the realization of the Haldane model and the photoinduced anomalous quantum Hall effect. Thanks to its high sensitivity to changes in the crystal symmetry, nonlinear optical spectroscopy provides an excellent tool to study these effects.

In our work, we use an elliptically polarized laser beam to excite monolayer graphene, where the circular polarization component breaks TRS. This symmetry breaking induces new nonzero elements in the third-order nonlinear susceptibility tensor, which are then probed by the linear component of the excitation beam. The combination of the already existing and the light induced tensor elements results in a rotation of the emitted third harmonic signal. Preliminary experimental results further indicate an impact of both excitation power and doping of the sample. Since SIS is still intact, our approach offers a new method for exploring broken TRS and topology in centrosymmetric materials.

HL 29.24 Tue 18:00 P1

Optical Probing of the K-Point Band Structure in Monolayer TMDs *via* SHG — •Jonas Margraf[1], Paul Herrmann[1], Sebastian Klimmer[1,2], Shridhar Sanjay Shanbhag[3], Jan Wilhelm[3], and Giancarlo Soavi[1,4] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]ARC Centre of Excellence for Transformative Meta-Optical Systems, Department of Electronic Materials Engineering, Research School of Physics, The Australian National University, Canberra, Australia — [3]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — [4]Abbe Center of Photonics, Institute of Applied Physics, University of Jena, Germany.

Crystal properties are ultimately defined by their band structure and dispersion relation, which are typically measured *via* angle-resolved photoemission spectroscopy. Recently, all-optical approaches based on non-perturbative nonlinear optics (NLO) have been proposed as a promising alternative. While optical probing of the band structure requires non-perturbative measurements of the entire Brillouin zone, it is often sufficient to probe the dispersion relation in the vicinity of optical resonances. In this work, we aim to measure the dispersion relation of a transition metal dichalcogenide monolayer at the ±K valleys using perturbative NLO. We investigate a modulation of the total second harmonic (SH) intensity as a function of the fundamental polarization angle upon two-photon resonant SHG. We assign this modulation of

the SH intensity to the specific dispersion relation of the ±K valleys induced by trigonal warping.

HL 29.25 Tue 18:00 P1

Optical properties of transition metal dichalcogenides under high pressure — •Paul Luca Grosserhode, Paul Steeger, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDCs), such as MoS_2 or WS_2, have received growing attention during the last years. Using micromechanical exfoliation, single semiconducting layers can be readily prepared. Furthermore, multi-layered artificial crystals can be fabricated with single layer precision. In this study, we use a diamond anvil cell to apply pressures in the gigapascal range on such samples and observe how their optical properties change due to the induced deformation.

HL 29.26 Tue 18:00 P1

Analytical Theory Of Third Harmonic Generation In Two-Dimensional Materials — •Shridhar Sanjay Shanbhag[1], Florentine Friedrich[2], Paul Herrmann[2], Giancarlo Soavi[2,3], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany

Valleytronics explores the valley degree of freedom in materials like transition metal dichalcogenides, using electrons in *K valleys as binary states for information encoding. In valleytronics, efficient valley readout is crucial, and third harmonic generation (THG) could provide an ultrafast solution to valley readout for any material, regardless of inversion symmetry.

We derived an analytical expression for THG by solving the semiconductor Bloch equations perturbatively to obtain an expression for the polarization state of the outgoing third harmonic. Our compact expression reveals how material parameters influence the polarization and attributes polarization rotation to valley-dependent optical Stark and Bloch-Siegert shifts. Our theoretical predictions closely align with experiments, providing the microscopic mechanism and thus helping to advancing valleytronic readout mechanisms.

HL 29.27 Tue 18:00 P1

Plasma-Induced Defect Emission in Hexagonal Boron Nitride — •Felix Schaumburg, •David Plitt, Timo Wagner, Nicolas Wöhrl, Martin Geller, Günther Prinz, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Hexagonal boron nitride (hBN) has been the subject of numerous research efforts in the last decade. Of particular interest is the creation of single emitters in hBN because of their easy integration, e.g. in van-der-Waals heterostructures, and their room temperature photon emission. Many methods to create single emitters in hBN are still under investigation. We present our approach to create single quantum emitters in hBN using a remote plasma with different plasma species. We have used argon, nitrogen, and oxygen plasmas and present statistics on the emitters, produced by the different gas species, and their optical properties. In particular, we examine the emission of the exfoliated flakes before the plasma processes *without* an annealing step to avoid creating emitters that are not caused by the plasma exposure. Our findings suggest that the purely physical argon plasma treatment is the most promising route for creating optically active single emitters in hBN by plasma exposure.

HL 29.28 Tue 18:00 P1

Single-photon emission in the van der Waals material hBN — •Akhilesh Dubey, Janne Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Single-photon sources are crucial components for quantum networks and communications. Recently, single-photon sources in 2D materials have emerged as robust solid-state light emitters. Promising materials include transition metal dichalcogenides, such as WSe_2, transition metal monochalcogenides (e.g. GaSe), and also hexagonal boron nitride (hBN). Here, we investigate the light emission from single-photon emitters in hBN. We measure photoluminescence spectra of individual centers in hBN nanocrystals and analyze their prominent phonon sidebands. Time-resolved photoluminescence measurements reveal typical lifetimes. Our results are important for devising novel nanoscale devices based on these robust quantum light emitters.

HL 29.29 Tue 18:00 P1

Spectroscopic investigation of defects in strained WSe_2 van-der-Waals heterostructures — •F. Stechemesser[1], F. Schaumburg[1], J. König[2], C. Dietrich[2], C. Steiner[3], P. Pesch[3], G. Prinz[1], M. Geller[1], and A. Kurzmann[2] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]University of Cologne, Physics Institute II, Germany — [3]2nd Institute of Physics, RWTH Aachen University, Germany

Van-der-Waals heterostructures offer a versatile platform for tailoring material properties through diverse layer compositions, making them suitable for a wide range of applications. We investigated the single photon emitting behavior of the Van-der-Waals heterostructure, that is composed of stacked layers containing graphene as a front and back gate, hexagonal boron nitride as dielectric layers and the transition metal dichalcogenide tungsten diselenide (WSe_2) as the host of optical emitters. The WSe_2 heterostructure was biaxially strained by nanopillars on the silicon wafer, which was used as substrate. By irradiating the points of large strain with an electron beam, point defects in the lattice structure of WSe_2 were created. The point defects, in the strained area, act as artificial atoms in the structure and can show single photon emission. We studied the samples using spacially resolved photoluminescence spectroscopy using a He-Ne laser. Applying this method, it is possible to localize an emitter and perform temperature, time and power dependent measurements. Finally, to prove the single photon characteristic of the emitter sites, we conducted second order correlation ($g^2(0) = 0.323$) measurements.

HL 29.30 Tue 18:00 P1

Tailoring Quantum Emission in Bilayer WSe2 via Strain Engineering — •Jasleen Kaur Jagde[1], Palwinder Singh[1], Grant Wilbur[1], Megha Jain[1], Edith Yeung[2], David Northeast[2], Seid Mohammad[2], Jean Lapointe[2], Dan Dalacu[2], and Kimberley Hall[1] — [1]Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Nova Scotia B3H 4R2, Canada — [2]National Research Council Canada, Ottawa, Ontario K1A 0R6, Canada

Two-dimensional semiconductors subjected to strain have shown exceptional promise as single-photon emitters, due to their direct bandgap and an ease of integration with photonic structures. Emitters have been observed in a host of monolayer (ML) materials including MoS2, WSe2, WS2, MoTe2 and hBN. Quantum emitters have also recently been discovered in bilayers of TMDs, however their optical properties are less well understood. In this study, we demonstrate site-selective quantum emission in bilayer (BL) WSe2 using strain localized by engineered dielectric nanopillars of varying diameters. Through a systematic investigation of the dependence of quantum emitter properties on strain, we determine the optimum conditions for the observation of bright and narrow photoluminescence emission peaks. We observe a strain-driven blue shift in the emission wavelength that is controllable by the characteristics of the nanopillar. A strong antibunching ($g(2)(0) = 0.139$) is observed, confirming single photon emission behavior. These results highlight strain engineering of 2D materials as a scalable strategy for on-demand quantum light sources.

HL 29.31 Tue 18:00 P1

Electrical impact of He ion broad beam irradiation on multi-layer WSe2 — •Madhuri Chennur[1,2], Zahra Fekri[1,2], Ulrich Kentsch[1], Gregor Hlawacek[1], Jens Zscharschuch[1,2], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328Dresden, Germany — [2]TUD Dresden University of Technology, 01062 Dresden, Germany

Nanoelectronics enables the development of innovative, cost-effective, miniaturized, and versatile materials. Among these, 2D materials hold immense potential for tailoring nanoscale functionalities. Structural defects in such materials play a significant role. By analyzing defect types, densities, and distributions, it is possible to unlock insights and exploit them for various applications, such as doping, tuning band gaps, or enhancing catalytic activity.

In this work, the impact of defects in multi-layer WSe2 is explored under the influence of Si/SiO2 and hBN substrates, introduced via a single broad-beam Helium ion irradiation at 7.5 keV. Electrical contacts are patterned using electron beam lithography (EBL), and

all measurements are conducted under ambient conditions to assess changes in defect states post-irradiation.

The evolution of defects is monitored over time, with observations made one and two weeks following irradiation. Initially, the devices demonstrate degraded performance but later, their current exceeds pre-irradiation levels. Raman spectroscopy before and after irradiation provides deeper insights into the material's behavior. Additionally, the findings reveal the role of defects in influencing gas-sensing capabilities.

HL 29.32 Tue 18:00 P1

Probing the Band Splitting near the Γ Point in the van der Waals Magnetic Semiconductor CrSBr — •Kaiman Lin[1,2], Yi Li[1,3], Mahdi Ghorbani-Asl[1], Zdenek Sofer[4], Stephan Winnerl[1], Artur Erbe[1,3], Arkady V. Krasheninnikov[1], Manfred Helm[1,3], Shengqiang Zhou[1], Yaping Dan[2], and Slawomir Prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Shanghai Jiaotong University, Shanghai, China — [3]TU- Dresden, Germany — [4]University of Chemistry and Technology Prague, Czech Republic

As a van der Waals magnetic semiconductor, CrSBr has a direct bandgap of approximately 1.5 eV and undergoes an antiferromagnetic transition around 131 K [1]. In this study, the electronic band structure of CrSBr is investigated through comprehensive photoluminescence (PL) characterization [2]. We distinctly identify low-temperature optical transitions between two closely adjacent conduction-band states and two different valence-band states. The analysis of the PL data robustly reveals energy splittings, bandgaps, and excitonic transitions across different CrSBr thicknesses, ranging from monolayer to bulk. Temperature-dependent PL measurements shed light on the stability of band splitting below the Néel temperature, suggesting that magnons coupled with excitons are responsible for the symmetry breaking and the brightening of transitions from the secondary conduction band minimum (CBM2) to the global valence band maximum (VBM1). [1] N. P. Wilson, K. Lee, J. Cenker et al., Nat. Mater. 20, 1657 (2021). [2] K. Lin, et al. J. Phys. Chem. Lett. 15, 6010-6016 (2024).

HL 29.33 Tue 18:00 P1

Tuning of non-radiative decay channels in CrSBr by a magnetic phase transition — •Fabian Glatz[1], Minjiang Dan[1,2], Till Weickhardt[1], Zdeněk Sofer[3], Marie-Christin Heissenbüttel[4], Julian Klein[5], and Giancarlo Soavi[1,6] — [1]Friedrich Schiller University Jena, Germany — [2]Southwest University of Science and Technology, Mianyang, China — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Westfälische Wilhelms-Universität Münster, Germany — [5]Massachusetts Institute of Technology, USA — [6]Abbe Center of Photonics, Jena, Germany

CrSBr is a layered magnetic semiconductor with a direct bandgap [1]. Magnetic measurements have shown that below the Néel temperature (132 K) the spins within a single layer arrange ferromagnetically, while multiple layers couple antiferromagnetically (AFM) [2]. Here, we investigate the evolution of CrSBr under a magnetic phase transition by using nonlinear optics. In agreement with existing literature, second harmonic generation (SHG) becomes allowed due to the symmetry-breaking by AFM ordering at low temperatures [3]. Additionally, this phase change from paramagnetic (PM) to AFM leads to a change in the band structure that enhances third harmonic generation (THG) at the lowest energy optical resonance while quenching the photoluminescence quantum yield. This indicates the opening of a phonon mediated non-radiative decay channel upon transition from PM to AFM phase.

[1] Wang et al., Nat. Commun. 14, 5966 (2023). [2] Telford et al., Adv. Mater. 32, 2003240 (2020). [3] Lee et al., Nano Lett. 21, 3511-3517 (2021).

HL 29.34 Tue 18:00 P1

Defect induced magnetic phase transition in CrSBr — •Fangchao Long[1,2], Mahdi Ghorbani-Asl[1], Kseniia Mosina[3], Joachim Thomsen[4], René Hübner[1], Zdenek Sofer[3], Florian Dirnberger[5], Arkady V. Krasheninnikov[1], Slawomir Prucnal[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Forschungszentrum Jülich, Germany — [5]Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

As an air-stable van der Waals magnetic semiconductor, CrSBr is receiving great research attention due to its exceptional properties. Below the Néel temperature of 132 K, CrSBr exhibits a typical A-type antiferromagnetic order comprised of antiferromagnetically coupled ferromagnetic monolayers. This special structure makes it susceptible to external stimuli, such as ion irradiation. In this work, we present the magnetic phase transition from antiferromagnetic to ferromagnetic in CrSBr crystals irradiated by non-magnetic ions. We observe the rise and fall of the ferromagnetic phase in antiferromagnetic CrSBr with increasing the irradiation fluence. Raman spectroscopy reveals phonon softening, suggesting the formation of defects. Structure analysis of the irradiated crystals in conjunction with density functional theory calculations suggest that the displacement of constituent atoms due to collisions with ions and the formation of interstitials favor a ferromagnetic order between the layers.

HL 29.35 Tue 18:00 P1

Self-Driven Photodetectors Based on Intercalated CrSBr — •Aljoscha Söll[1], Kseniia Mosina[1], Martin Vesely[1], Jiří Šturala[1], Florian Dirnberger[2], and Zdeněk Sofer[1] — [1]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic. — [2]Department of Physics, Technical University of Munich, 85748 Munich, Germany.

The intercalation of lithium ions into layered materials has been an important field of research, leading not only to the development of lithium-ion batteries but also to countless insights in solid-state physics. Recently, it was shown that the intercalation of the quasi-1D semiconductor CrSBr can drastically alter its electronic structure, enhancing conductivity and potentially causing a transition from semiconductor to metal. Since the location and degree of intercalation can be precisely controlled, it allows us to fabricate devices using partially or fully intercalated CrSBr, harnessing properties of both the pristine and intercalated phases. Here we present a self-driven photodetector based on intercalated CrSBr, demonstrating high photoresponsivity across the entire NUV to NIR range with a response time in the millisecond range. Our findings not only deepen the understanding of intercalation effects in low-dimensional materials but also pave the way for the development of advanced optoelectronic devices using intercalated CrSBr.

HL 29.36 Tue 18:00 P1

Strong coupling of metal nanoparticles and 2d semiconductors: Physics behind a minimal model — •Lara Greten and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Transition metal dichalcogenide monolayers (TMDCs) feature strong light-matter interaction, governd by tightly bound, 2d-delocalized excitons. Metal nanostructures exhibit localized plasmons allowing for extreme electric field enhancements on the nanoscale. Hybrids of TMDCs and metal nanoparticles combine excitons and plasmons and may reach strong coupling as shown in numerous experiments. These experimental results are typically quantified via the coupled oscillator model (COM) employing a phenomenological coupling constant as a fitting parameter. To provide physical background to this model, we develop an analytical theory based on a microscopic perspective of the material dynamics and Maxwell's equations [1]. The emergent minimal model [2] provides a clear physical interpretation that highlights the importance of the spatial dispersion of 2d excitons. Depending on geometry and material properties we derive analytic expressions for all coupling and dephasing constants in a COM combining three oscillators: plasmons, bright and momentum-dark excitons. Strong coupling, that manifests as a peak splitting in optical spectra, is observed between momentum-dark excitons and plasmons, while the weakly coupled bright exciton yields a distinct third peak.

[1] L. Greten et al., ACS photonics 11.4, 1396-1411 (2024)
[2] L. Greten et al., arXiv preprint arXiv:2410.16796 (2024)

HL 29.37 Tue 18:00 P1

Non-Local Effects in Landau Quantized Two-Dimensional Electron Gases — •Sabrina Meyer[1], Andreas Knorr[1], Stephen Hughes[2], and Lara Greten[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

Landau levels are the quantum analogon of the cyclotron motion under a strong magnetic field in two-dimensional electron gases, as present in high quality GaAs films. Even though recent experimental work examines nanopatterning - introducing metal gaps to localize and amplify electric fields on the nanoscale - current theoretical descriptions still rely on a local susceptibility for excitation with large wavelengths.

This study includes non-local effects in a microscopic theory for the electron dynamics: We find modified selection rules beyond the dipole approximation that allow for the direct excitation of ground state electrons to higher Landau levels, that are forbidden in a local description. These modifications become especially important when the electric field varies significantly within the spatial extend of the Landau level wave function ($\propto$ 100 nm). This applies for nanopatterned devices as well as for light scattering with wavelength on the order of the Landau level radius.

HL 29.38 Tue 18:00 P1

Visualizing Atomic-Scale Charge Fluctuations in Real-Space Dielectric Response — •Bernadette Christ and Claudia Rödl — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The wave-vector and frequency-dependent dielectric function contains a plethora of information on the response of a given material to external perturbing electromagnetic fields that is rarely fully exploited. Its off-diagonal elements are known as local-field effects and encode the atomic-scale charge fluctuations that occur due to light-matter interaction or screening within the material.

We aim for developing a tool to visualize the impact of such an external perturbation on the electron density in the material in real space. In a first step, we calculate the independent-particle dielectric response function from first principles using density-functional theory. In this mean-field approach, we expect to see how interband transitions excite individual orbitals and how collective excitations such as plasmon waves propagate in the material. Later on, we will also consider inclusion of many-body effects in the evaluation of the response function to visualize the formation of excitons. This will help us to better understand the intricate interplay between the numerous electronic degrees of freedom and contribute to the analysis of spectroscopic experiments. As first benchmarks, we will study bulk semiconductors heading for more complex, technologically relevant materials systems afterwards.

HL 29.39 Tue 18:00 P1

Assessing Wafer Growth Success in Quantum Dot Photonic Device Fabrication — •Severin Krüger[1,2], Elias Kersting[1], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Sparrow Quantum Aps, Copenhagen, Denmark

Molecular beam epitaxy (MBE) is crucial for fabricating photonic devices, including commercially viable single photon sources (SPS) based on quantum dots (QDs) [1]. Precise control of QD properties and surrounding layer design is essential for optimal device performance. We employ bandstructure and photonic simulations to design heterostructures, followed by comprehensive optical characterization of reference samples using photoluminescence (PL) mapping, Hall measurements, and surface analysis. This efficient characterization cycle allows rapid optimization of growth parameters on full 3" wafers, significantly reducing development time compared to direct SPS fabrication and testing. However, distributed Bragg reflectors in SPS wafers introduce PL signal artifacts due to reflectivity oscillations and stop bands, which significantly modulate the collectable photon yield across different wavelengths, alternately enhancing and suppressing the signal. We present our reference sample approach, characterization methods, and techniques to correct for optical stack-induced PL artifacts, enabling accurate assessment of MBE-grown structures for SPS applications.

[1] R. Uppu et al., Nature Technology 16, 1308-1317, (2022) [2] H.G. Babin et al., Nanomaterials 11, 2703, (2021)

HL 29.40 Tue 18:00 P1

Effect of TiO_2 thin films on the charge state of shallow NV centers in diamond. — •Arthur Witte, Tobias Lühmann, Peter Schlupp, Dominic Reinhardt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute for Solid State Physics, Germany

The nitrogen vacancy (NV) center is a color center in diamond. In its negative charge state, it has a relatively long spin coherence time at room temperature and a spin-dependent photoluminescence that enables optical spin polarization. Because of these properties, the NV center was proposed as a platform for room-temperature quantum computing. For this application the NV centers must be located close to the diamond surface. This can present new challenges due to surface effects resulting in, e.g. charge state instabilities of the shallow NV centers. Various surface treatments can be used to mitigate these effects, such as thermal oxidation, plasma surface treatments or the deposition of a thin passivation layer on the diamond surface.

We present a titanium dioxide thin film as the passivation layer. Titanium dioxide is a wide-bandgap semiconductor with a high refractive index of 2.5. In a first step, we investigate the growth of titanium dioxide layers by pulsed laser deposition and long-throw sputtering under different conditions. We then study the effect of optimized titanium dioxide layers on the luminescence properties of NV centers at implantation depths between 7 nm and 67 nm. Through spectroscopic analysis, we observe a significant increase in charge stabilization of shallow NV centers.

HL 29.41 Tue 18:00 P1

Secondary electron spectrometer for deterministic single ion implantation — •Priyal Dadhich, Nico Klingner, and Gregor Hlawacek — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf(HZDR), Dresden, Germany

The deterministic placement of single ions is essential for programmable quantum computers based on the nuclear spin of the donor atom to serve as a spin qubit.

Spatially revolved single ion implantation requires the reliable detection of implantation events. Our approach utilizes SEs generated during ion impact. To optimize the detection we use a windowless silicon drift detector (SDD) biased up to +10 kV. The SDD measures the electron energy through electron-hole pair generation, enabling quantifying the number of electrons by counting pile-up pulses [1]. Given the low average SE yield per single-ion impact, optimizing the extraction geometry is crucial for achieving the maximum possible success rate.

We use the open-source three-dimensional ion optical C++ library, IBSIMU[2], to simulate a realistic extraction design for efficient SE collection on the detector's active area. For the highest detection efficiency, we must also consider the unlikely event of backscattering of the electrons from the SDD. The extraction geometry is designed to recapture these electrons and re-accelerate them into the detector's active area.

[1] F. Aumayr et. al., Applied Surface science,47(2):139*147, 1991.
[2] Taneli Kalvas et. al., Review of Scientific Instruments, 81(2), 2010.

HL 29.42 Tue 18:00 P1

Emission properties of electron irradiated hBN — •Annkathrin Köhler, Jan Böhmer, Christian T. Plass, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Defect centers in solid state materials have emerged as promising candidates for quantum emitters. In particular, hexagonal boron nitride (hBN) has attracted significant attention due to its ability to host single-photon emitters (SPEs) at room temperature. Here, we systematically examined the luminescence properties of exfoliated hBN flakes as well as hBN nano-powders dispersed in various solutions and drop-casted onto a substrate. The effects of local electron irradiation and thermal annealing on the hBN samples were analyzed, providing insights into the conditions necessary for tuning their emission characteristics. Photoluminescence (PL) spectra were recorded using a micro-PL setup to compare the spectral distribution of the emission under different treatments. To further understand the quantum nature of the emitters, we conducted second-order correlation measurements as a function of the preparation parameters.

HL 29.43 Tue 18:00 P1

Germanium MOSFETs for Quantum Computation — •Thembelihle Dlamini and Mónica Benito — Institute of Physics, University of Augsburg

The project focuses on studying hole dynamics and spin properties in Germanium (Ge) metal-oxide-semiconductor (MOS) nanostructures to achieve high-fidelity single-qubit operations. Leveraging MOSFETs superior compatibility with industrial manufacturing techniques, holes' unique properties such as strong spin-orbit coupling, and Ge advantages over Si, GeMOS hole-spin qubits addresses some of the limitations of state-of-the-art spin quantum processors. The device-design phases will be assisted by three-dimensional structural simulations of the device. Moreover we will develop custom analytical models for holes in low-dimensional GeMOS geometries and the Ge/oxide interface by using symmetry analysis and $k \cdot p$ theory. Finally, we will investigate the effect of the multiband character of holes and their spin-orbit coupling in the effective spin representation of systems with a few holes in realistic quantum-dot potentials.

HL 29.44 Tue 18:00 P1

Crystal Growth and Influence of Fe^{3+} Doping on the Structural, Optical, and Magnetic Properties of Lead-Free Double Perovskites — •Volodymyr Vasylkovskyi[1,2], Anastasiia Kultaeva[1], Olga Trukhina[1], Patrick Dörflinger[1], Daniele Ludwig[1], Mykola Slipchenko[1,2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Institute for Scintillation Materials, NAS of Ukraine, 61072 Kharkiv, Ukraine

Semiconducting perovskite materials have attracted significant attention for their photovoltaic and light-emitting applications, yet their magnetic properties are largely unexplored. Doping perovskites with transition metal ions, such as Fe^{3+}, introduces novel properties, broadening their potential for spintronic and quantum applications.
In this study, Fe-doped $Cs_2AgBiBr_6$ and $Cs_2AgBiCl_6$ single crystals were synthesized using a controlled cooling crystallization technique with varying Fe^{3+} doping concentrations. Despite low Fe^{3+} incorporation (<0.01%), doping significantly affected defect density, optical properties, and magnetic behavior. Electron paramagnetic resonance revealed complex spin properties of the intrinsic spin centers and their interactions, which depend on both temperature and the orientation of single crystals with respect to the magnetic field.
Our findings highlight Fe-doped lead-free perovskites as promising materials for spintronic applications, emphasizing the importance of precise doping and defect manipulation to optimize their performance.

HL 29.45 Tue 18:00 P1

Multi-Frequency ODMR applied to Boron Vacancy Spin Defects of hBN — •Lucas Schreiber, Selin Steinicke, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Spin defects in hexagonal boron nitride (hBN) present a multitude of potential applications in the fields of quantum sensing and quantum information technology. Especially, the negatively charged boron vacancy defect can interact with the nuclear spins of its surrounding nitrogen atoms, thereby giving rise to hyperfine interactions. In this study, the spin defect was analyzed using optically detected magnetic resonance (ODMR) spectroscopy, wherein the spin sublevels are controlled by microwave pulses. In contrast to previous studies, the coherent microwave pulses employed in this work simultaneously utilize the multiple resonance frequencies of the hyperfine splitting. We therefore implement a multi-resonance technique for enhanced contrast and exploitation of the spin system. For an accurate and quantitative comparison with conventional ODMR, we derived a value for the contrast, allowing for a direct comparison of the hyperfine interaction on the spin defect. This approach aims at enhancing the optical detection of resonant excitation of the spin defect and facilitating coherent control experiments in future studies.

HL 29.46 Tue 18:00 P1

Temperature-dependent Studies of Boron-Vacancy Spin Defects in hexagonal Boron Nitride — •Selin Steinicke, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Optically addressable spin-carrying defects in solid-state materials are promising candidates in the field of quantum information technology and sensing applications. The recently discovered negatively charged Boron vacancies (V_B^-) in hexagonal Boron Nitride (hBN) raised the prospect of quantum sensing in a two-dimensional material. Although numerous studies on hBN emerged in the last years, the optical pump cycle has not yet been fully researched. Temperature-dependent spectroscopy on V_B^- ensembles shows broad photoluminescence around 850 nm and an increase in intensity at cryogenic temperatures. Using temperature-dependent transient photoluminescence measurements, we investigate the non-radiative relaxation path from the triplet excited state into the triplet ground state via the metastable intermediate state. The dependence of the intermediate state's lifetime on temperature is examined. These results shed light into the dark processes of V_B^- and can be used to optimize coherent control of V_B^-, which leads to a higher sensitivity in quantum sensing.

HL 29.47 Tue 18:00 P1

Investigating the optical pumping of silicon vacancies in 4H-SiC to increase the maser output — •Emilian Eisermann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

A major breakthrough in the realization of a continuous-wave maser at room temperature was achieved with the utilization of nitrogen vacancies in diamond. However, diamond is a comparatively expensive material. For this reason, silicon carbide (SiC), a material used commercially in electrical systems, has received attention in recent years. Only recently, our group has demonstrated the first room temperature continuous-wave SiC maser. Despite innovative microwave feedback loop engineering, only a low output could be achieved. In an effort to boost the maser output, we investigate the fundamental pumping behavior of silicon vacancy defects in SiC in dependence of the optical pump wavelength, the temperature and their density. Using electron paramagnetic resonance spectroscopy, we resolve microwave absorption and emission signals due to the optical polarisation of Zeeman-split states. By analyzing these features, we calculate the population inversion in the gain material. This crucial parameter allows us to quantitatively evaluate the pump efficiency. It turns out that an excitation with an energy of the zero-phonon line of the silicon vacancy is particularly efficient. Furthermore, we examine to what extent excitation with an energy lower than that of the zero-phonon line is possible if thermally driven phonons are used to compensate the missing energy. First results are presented on the poster, which we are discussing here.

HL 29.48 Tue 18:00 P1

UV Photolithographic Fabrication of Photonic Structures on Diamond — •Nidhin Varghese, Oleg Peter, and Wolfgang Harneit — Institute of Physics,University of Osnabrück,Germany

The NV center in diamond is a point defect with promising quantum applications at room temperature, combining long spin relaxation times with optical excitation and state readout. Photonic structures such as micron-sized pillars help to increase the photon collection efficiency, improving the SNR ratio and enhancing sensitivity. NV centers in photonic structures can also be used to read out and control other spins, e.g., molecular qubits The top-down approach to fabricating photonic structures is straightforward and based on reactive ion etching of diamond. The process first requires a patterned etching mask, which is usually defined using electron beam lithography (EBL). Although EBL allows to make very small patterns, it is quite expensive and time-consuming. Using photolithographic processes could enhance industry adoption and increase accessibility to diamond quantum technology for research labs that do not have access to EBL. Here, we present a novel approach to nano-pillar fabrication based on direct (UV) laser writing lithography. An easy-to-use epoxy stage was developed for spin coating of photoresists on very small substrates, which largely supresses the formation of edge beads. The photonic pillar structures were fabricated by lithography and ion etching, and characterized. Confocal fluorescence scans demonstrated the increased photon output performance. CW-ODMR measurements confirmed the presence and accessibility of NV centers.

HL 29.49 Tue 18:00 P1

Birefringence effects in crystalline AlGaAs/GaAs mirror coatings from 4 K to room temperature — •Mona Kempkes, Chun Yu Ma, Thomas Legero, Uwe Sterr, and Daniele Nicolodi — Physikalisch-Technische Bundesanstalt, Braunschweig

Coating thermal noise limits the performance of high precision interferometry experiments, including ultra-stable optical oscillators used for interrogating atomic clocks and gravitational wave detectors. Due to their low mechanical losses, Bragg-reflectors from crystalline $Al_{0.92}Ga_{0.08}As$/GaAs heterostructures emerged as a lower thermal noise alternative to traditional dielectric mirror coatings. Mirrors realized with this material exhibit still poorly understood birefringence that can be modified by temperature and incident optical power. Furthermore, experiments at 4 K, 16 K and 124 K revealed spontaneous fluctuations of the birefringence, as well as an additional and yet unidentified noise source that limits the performance well above the expected thermal noise floor [J. Yu et al., Phys. Rev. X 13, 041002 (2023)]. Reconciling these observations from different samples is challenging and hinders a common interpretation. Thus we have set up one system where the temperature can be swept continuously across a wide range. We will present our setup based on a low-vibration closed-cycle cryostat, and measurements of the birefringence of crystalline AlGaAs/GaAs mirror coatings from 4 K to room temperature and as function of optical power.

HL 29.50 Tue 18:00 P1

Stark Effect of color centers studied from a- and m-face 4H-SiC — •Fabio Candolfi, Johannes A. F. Lehmeyer, Michael

Krieger, and Heiko B. Weber — Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Angewandte Physik, Staudtstr. 7 91058 Erlangen, Germany

Color centers in silicon carbide (SiC) can operate as single photon sources and are well suited for photonic quantum technology. As compared to the intensively studied diamond platform, SiC provides both mature semiconductor functionality and process technology.

We investigated the Stark effect response of two different color centers in 4H-SiC; the established silicon vacancy defect and the less known TS defect. Both were studied from the c-face, but the photon emission occurs predominantly in the basal plane. This is why in this work low-temperature photoluminescence across the a- and m-faces were studied with Stark effect along three principal crystallographic axes. From the emission polarization of shifted and split photoluminescence lines we obtain the orientation of the dipole moment.

HL 29.51 Tue 18:00 P1

InGaAs quantum dots grown by local droplet etching — •Selma Delić[1,2], Xuelin Jin[1,2], Nils von den Driesch[1], Elias Kersting[3], Arne Ludwig[3], Alexander Pawlis[1], Detlev Grützmacher[1,2], and Beata Kardynal[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, RWTH, 52074 Aachen, Germany — [3]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Gallium arsenide quantum dots (QDs) grown using local droplet etching epitaxy (LDE) have been shown to be excellent single photon emitters. Integrated into GaAs heterostructures with two-dimensional electron gases (2DEG), the LDE QDs could facilitate spin-photon interface to spin-qubits in gated QDs, provided that photon absorption in the 2DEG in eliminated.

In this contribution, we demonstrate that the wavelength of LDE quantum dots can be effectively tuned by filling the holes edged in Al0.33Ga0.67As with InxGa1-xAs with x=10-20%. At such compositions, two-dimensional growth is expected and quantum dot formation should follow the same mechanism as that of GaAs QDs. We characterise the QDs using atomic force microscopy, low-temperature photoluminescence (PL), and microPL and analyse the effects of the growth temperature, etching step parameters, and filling material on the wavelength of QD emission. Furthermore, we show how the wetting layer emission wavelength can be used to evaluate the thickness and composition of the deposited InxGa1-xAs.

HL 29.52 Tue 18:00 P1

Tuning InGaAs quantum dots for quantum interface for heterogeneous quantum network — •Xuelin Jin[1,2], Selma Delic[1,2], Zheng Zeng[1,2], Nils von den Driesch[1,3], Alexander Pawlis[1,3], Detlev Grützmacher[1,2,3], and Beata Kardynal[1,2] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen, 52074 Aachen, Germany — [3]Peter Grünberg Institute 10, Forschungszentrum Jülich, 52425 Jülich, Germany

Abstract. Connecting different spin qubits using photonic qubits could facilitate building networks that would benefit from the inherent advantage of the individual subsystems. An efficient transfer of a qubit from a photon to the spin qubit requires matching of the energies and the bandwidths of the photon wave packet and the spin qubit optical transitions.

We discuss the design of an epitaxial quantum dot device that aim to use electrostatic gates to manipulate the bandwidth of the photons emitted from InAs QDs to improve the match to the spin qubits realized in trapped ions. We show that application of electrostatic fields can change the overlap of the e-h wavefunctions. We will discuss the conditions that the heterostructure has to fulfill for the device operation and will show the status of fabrication, which has centered on optimizing the epitaxial growth of the material. Finally, we will show the results of its characterisation aiming to show how the electronic states in these quantum dots evolve with voltages applied to the surface gates.

HL 29.53 Tue 18:00 P1

Spin-Dependent Processes Involving Defects Caused by Lithography — •Henry Stock[1,3], Michael Göldl[1,3], Niklas Bruckmoser[2,3], Leon Koch[2,3], Stefan Filipp[2,3], and Martin S. Brandt[1,3] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Straße 8, 85748 Garching, Germany — [3]School of Natural Sciences, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany

A precise knowledge of the paramagnetic defects present in quantum devices and their contribution to magnetic noise can be crucial for the optimization of such devices. However, conventional electron spin resonance experiments are often not sensitive enough to observe the defects. Using spin selection rules governing, e.g., recombination, the sensitivity of magnetic resonance experiments can be improved significantly. In its pulsed form, this so-called electrically detected magnetic resonance (EDMR) even enables the time-resolved study of the spin dynamics of the defects, allowing for measurements of the formation and recombination of spin pairs, as well as of the spin relaxation times T_1 and spin decoherence times T_2. Here, we present a study where we investigate paramagnetic P_{b0} defects and lithographically induced fluorine defects in Si substrates used for the manufacturing of superconducting transmon qubits. Our results are important to illuminate the role these defects play in flux noise and their influence on qubit coherence.

HL 29.54 Tue 18:00 P1

Progress on fully gate-defined optical interfaces to spin qubits — •Maxim Reznikov[1], Sebastian Kindel[1], Kui Wu[2], Nikolai Spitzer[3], Andreas D. Wieck[3], Arne Ludwig[3], Jeremy Witzens[2], and Hendrik Bluhm[1] — [1]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Germany — [2]Institute of Integrated Photonics, RWTH Aachen University, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Advancing quantum networks beyond proof-of-concept applications requires an approach for fabricating quantum repeater nodes with multiple qubits and optical interfaces in a controlled manner. Semiconductor spin qubits in gate-defined quantum dots address these needs in terms of established high-fidelity qubit operations and compatibility with industrial semiconductor technology. By employing electrostatic gating on either side of a submicron-thick heterostructure, excitons can be precisely localized at deterministic positions, thus also realizing an optical interface. These exciton trapping devices overcome the fabrication randomness associated with self-assembled quantum dots and enabling fine-tuning of operational wavelengths.

In this work, we demonstrate the successful integration of exciton trapping devices based on GaAs quantum wells into photonic crystal cavities. Additionally, we show the same confinement mechanism can be transferred to the Ge/SiGe platform, which is more compatible with industrial processing and telecom wavelength.

HL 29.55 Tue 18:00 P1

RPCVD growth of nuclear spin-free 70Ge/28Si70Ge heterostructures on industrial SiGe wafers — •Patrick Daoust, Simone Assali, Anis Attiaoui, Gérard Daligou, Patrick Del Vecchio, Sebastian Koelling, Lu Luo, Nicolas Rotaru, Oussama Moutanabbir, and Éloise Rahier — Department of Engineering Physics, École Polytechnique de Montréal, C.P. 6079, Succ. Centre-Ville, Montréal, Québec, Canada H3C 3A7

The coherence and operation of hole spin qubits in planar Ge heterostructures are both very sensitive to the nuclear spin bath. Therefore, developing nuclear spin-depleted materials is critical to control the performance of these quits. To this end, it is important to eliminate the nuclear spin-full 29Si and 73Ge in the epitaxial Ge/SiGe heterostructures. Our group has recently demonstrated highly crystalline, defect free, isotopically purified (>99.9 at.% 70Ge) nuclear spin-depleted 70Ge quantum well (QW) heterostructures grown in a reduced pressure CVD using purified precursors (>99.9 at.% 70GeH4 and >99.99 at.% 28SiH4) on in situ grown reversed graded SiGe buffers [1]. However, this growth protocol is not efficient and consumes significantly these purified precursors. Herein, we show that the growth of 70Ge QW can be achieved on industrial SiGe wafers thus optimizing the usage of precursors, preventing any background contamination from natural precursors, and yielding highly purified 70Ge/28Si70Ge heterostructures.

HL 29.56 Tue 18:00 P1

Time resolved electron imaging of a high-Q nonlinear nanomechanical oscillator — •Kai Nettersheim[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

While micro-electromechanical systems are well adapted for probing nonlinear dynamics in nanomechanical systems, they are often limited in their spatial resolution. Recent advances in ultrafast electron microscopy (UTEM) [1] enable the highly localized probing of nanoscale oscillator dynamics as well as their atomic structure and material defects.

Here, we present the characterization of non-linear free-standing silicon membranes by UTEM imaging techniques using an event-based electron detector with nanosecond temporal resolution. By exiting the sample with a modulated continuous wave laser the sample is driven into the nonlinear regime, resulting in Duffing resonances with high quality factors of up to 10^5. We experimentally characterized the temperature and fluence dependencies of the resonance as well as the mode shapes involved and compare these to finite-element simulations.

[1] A. Schröder et al., arXiv:2410.23961v1 (2024)

HL 29.57 Tue 18:00 P1

Quantum Particles on Strongly Bent Curves — •Tim Bergmann, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

Quantum systems under geometrical restrictions appear both in research and applied fields such as materials design, for example in the context of quantum wires. In the case of a curve these lead to a one-dimensional Schrödinger equation with its curvature appearing as a potential like term. Up to this point, there existed no ansatz for the treatment of singulary bent curves because the curvature diverges. We provide a solution to this problem for a subclass of such curves, employing a useful mathematical tool for the convergence of eigenvalue equations. This desingularization renders the approximation of the eigenspectrum and corresponding wave functions of systems with singular Hamilton operators possible.

HL 29.58 Tue 18:00 P1

Shutter synchronized deposition in molecular epitaxy for wafer scale homogeneous quantum emitter growth — •Elias Kersting, Hans Georg Babin, Nikolai Spitzer, Andreas Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

Most quantum dot (QD) based single photon emitters today are based on random position nucleated QDs with spectrally broad emission properties. Deterministic QD growth in position and emitter wavelength would be highly appreciated for large-scale and good turnabout chip manufacturing. Local droplet etching during molecular beam epitaxy is an all-in-situ method to predetermine the nucleation site of quantum dots. As recently demonstrated, this method can produce strain-free GaAs QDs with excellent photonic and spin properties. We use random position droplet nucleation and hole filling demonstrating enhanced emitter wavelength homogeneity on a wafer scale. By shutter synchronized rotation and ideal growth parameters, we grow QDs with a peak emission wavelength spread of no more than 2 nm on a full 2" diameter area with a narrow inhomogeneous ensemble broadening. While the emission wavelength of these QDs is < 800 nm, we can use this random local droplet nucleation, nanohole drilling and InAs infilling to produce QDs emitting in the telecom optical fibre transparency window around 1.3 μm, the so-called O-band. For this approach, we demonstrate 2" wafer scale control of the emission wavelength and excellent uniformity. We discuss our methodology, structural and optical properties.

HL 29.59 Tue 18:00 P1

Integration of quantum dot-based single-photon sources onto silicon photonic platform using micro-transfer printing — •Simon Oberle, Ponraj Vijayan, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Germany

Silicon photonics for telecommunications applications has garnered much attention recently. The optical transparency and the large refractive index contrast of silicon in the telecommunication wavelengths allow the implementation of high-density photonic integrated circuits. One disadvantage of silicon photonics is the lack of a native light source due to the indirect band-gap nature of silicon. One potential solution is the integration of III-V material, which offers outstanding optical emission properties, on a silicon platform. The direct growth of III-V materials on silicon is economically favourable and therefore the most desired approach. However, it is challenging because of the large lattice mismatch between the III-V materials and silicon. An alternate approach for large-scale integration is through hybrid integration of III-V structures using micro-transfer printing. Our group has previously developed In(Ga)As quantum dots on GaAs emitting in the telecom C-band. Here, we report our approach to designing and fabricating structures for the hybrid integration of these QDs onto a silicon platform using micro-transfer printing.

HL 29.60 Tue 18:00 P1

enhancing the emission Intensity of Mn2+ by doping with Ln3+ ions in ZnSe QDs and heavy metal ions detection — •Iram Gul[1], Zahid U. Khan[2], Latif U. Khan[3], Hermi F. Brito[4], and Muhammad Abdullah Khan[5] — [1]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan — [2]Research Centre for Greenhouse Gas Innovation, University of Sao Paulo (USP), 05508-030, São Paulo * SP, Brazil — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan — [4]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [5]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan

This study enhances the photoluminescence of ZnSe:Mn2+ quantum dots (QDs) by doping with Ln3+ ions (Sm3+, Gd3+, La3+, Y3+, Nd3+, Yb3+, Tm3+, Lu3+). Sm3+ and Gd** exhibited the strongest emissions due to efficient energy transfer to Mn2+, while other ions showed quenching at higher concentrations. These QDs, with uniform morphology, were applied to detect heavy metals (Pb2+, Cr3+, Hg2+, Cu2+, Fe2+), which quenched photoluminescence. Pb2+ showed the highest sensitivity (LoD: 4.648.10-3 mol/L), and Fe2+ the lowest (LoD: 5.257.10 -3 mol/L). ZnSe:Ln3+,Mn2+ QDs demonstrate potential for advanced photoluminescent applications and environmental monitoring of pollutants

HL 29.61 Tue 18:00 P1

enhancing the emission Intensity of Mn2+ by doping with Ln3+ ions in ZnSe QDs and heavy metal ions detection — •Iram Gul[1], Zahid U. Khan[2], Latif U. Khan[3], Hermi F. Brito[4], and Muhammad Abdullah Khan[5] — [1]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan — [2]Research Centre for Greenhouse Gas Innovation, University of Sao Paulo (USP), 05508-030, São Paulo SP, Brazil — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan — [4]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [5]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan

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HL 29.62 Tue 18:00 P1

Towards Efficient Entangled Photon Pair Sources by Semiconductor Quantum Dots in Planar Cavities — •Aditi Javali[1], Raphael Joos[1], Ponraj Vijayan[1], Lena Engel[1], Tobias Huber-Loyola[2], Sven Höfling[2], Michael Jetter[1], Simone Luca Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Lehrstuhl für Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Since the EPR violation, entangled photons have become key protagonists in quantum technology, serving as communication carriers via polarization qubits. Photon pairs entangled in telecom C-band are particularly advantageous, as this wavelength range minimizes dispersion and loss in standard optical fibers, enabling long-distance communication with reduced signal degradation. In this work, we demonstrate the generation of entangled photon pairs in the telecom C-band using InAs quantum dots integrated with a planar photonic cavity. The cavity enhances photon emission rates and collection efficiency with high entanglement fidelity. The biexciton state, emitting the entangled pair,

is prepared using a two-photon excitation scheme. The entanglement is verified through state tomography, confirming the strong quantum correlations between the photons. This work highlights telecom C-band quantum dots' potential as efficient entangled-photon sources for high-performance quantum communication.

HL 29.63 Tue 18:00 P1

Influence of Short-Wavelength Irradiation on Self-Assembled Quantum Dots — •Julia Avdeev[1], Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Charlotte Rothfuchs-Engels[2], Sven Scholz[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

Using Deep Level Transient Spectroscopy (DLTS) the charge transfer to and from Self-Assembled Quantum Dots (SAQDs) at large distance from the reservoir can be observed. Measurements are performed at a temperature of 77 K studying the influence of short-wavelength infrared irradiation. With wavelengths larger than 1.5 μm photons are not capable to induce charge emission from neutral Quantum Dots in ground state but can cause free charge carriers from electronic states in SAQDs.

HL 29.64 Tue 18:00 P1

Quantum Mechanics on Periodically Deformed Manifolds — •Theresa Appel, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Deutschland

Quantum systems confined to low-dimensional geometries exhibit unique physical behavior due to curvature-induced potentials. The poster presents results on the dynamics of particles confined to periodically curved manifolds, which we term "deformation crystals". The periodic spatial deformations directly influence the particle dynamics resulting in a band structure similar to other crystalline systems. We examine the transition from a free electron gas to a one-dimensional deformation crystal while analyzing the energy dispersion relation and symmetry-breaking effects. Furthermore, the behavior of different deformations is compared. The results reveal that the specific geometric deformations significantly influence the effective potential landscape and the band structure, thus opening up new opportunities for applications via deformation modulation of the underlying space.

HL 29.65 Tue 18:00 P1

Single-electron charging events on quantum dots in InSb nanowires — •Marcus Liebmann[1], Kanji Furuta[1], Sasa Gazibegovic[2], Diana Car[2], Erik Bakkers[2], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Dept. of Appl. Phys., Eindhoven Univ., The Netherlands

As a first step to realize a single-electron counting tip for a scanning tunneling microscope, we investigate the charge state of a quantum dot (QD) by recording the current through a floating-gate-coupled sensor dot. InSb nanowires are placed mechanically onto bottom gates with hexagonal boron nitride (h-BN) as a dielectric to define two quantum dots capacitively coupled via a floating gate. At zero source-drain voltage and high barriers, charge stability diagrams are acquired, and time series of the QD charge state reveal single-electron charging events. These are analyzed with respect to full counting statistics. The Fano factor and factorial cumulants [1] are extracted to search for correlation effects.

[1] P. Stegmann *et al.*, Phys. Rev. B **92**, 155413 (2015).

HL 29.66 Tue 18:00 P1

Spin relaxation dynamics of the excited triplet state in self-assembeld quantum dots — •Carl Nelson Creutzburg[1], Jens Kerski[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The two-electron triplet state in a self-assembled quantum dot (QD) can pair with the singlet ground state to form a spin qubit. This state is electrically addressable, making it a promising candidate for quantum information processing. Achieving this requires a long coherence time (T_2), which is limited by the spin relaxation time (T_1). While T_1 has been previously studied using optical techniques, we employ an all-electrical measurement approach. The dots are embedded in an inverted high electron mobility transistor (HEMT) to selectively charge and discharge their many-particle states with electrons from a tunnel-coupled electron reservoir (2DEG). The 2DEG also acts as a sensitive detector for the charge in the QD layer. By employing time-resolved transconductance spectroscopy [1] and varying the charging intervals, we observe the relaxation process from the excited triplet state to the singlet ground state. Using a rate equation model, we extract the spin relaxation time T_1. While there are already first results for T_1 [2], an improved temporal resolution provides new insights that could help to refine assumptions in previous studies.

[1] B. Marquardt. et al., Nature Commun. 2, 209 (2011)
[2] K. Eltrudis. et al., Appl. Phys. Lett. 111, 092103 (2017)

HL 29.67 Tue 18:00 P1

Multiphoton Emission of Quantum Dots with Different Excitation Schemes — •Patricia Kallert, Nicolás Claro-Rodríguez, Francesco Salusti, Sonja Barkhofen, Santiago Bermúdez Feijóo, Lukas Hanschke, Normen Auler, Dirk Reuter, and Klaus D. Jöns — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany

High efficiency, single-photon purity, high indistinguishability, and good qualities as entangled-photon pair emitters are key properties of ideal sources for photon-based quantum technologies. Accordingly, semiconductor quantum dots (QDs) are promising candidates. If a multi-level system is excited coherently with optical pulses of different pulse areas, such as 1π, 2π and higher, the system experiences Rabi rotations of the according rotation and the respective population inversions. For each pulse area, the probability of emitting different photon numbers for different pulse areas varies, which is recognizable in the second correlation function. [1] Since various excitation schemes are interesting for different qualities of QDs, we analyze the multiphoton emission characteristics with different excitation schemes. We anticipate that this gives a deeper insight into the structure of the emitted states and possible applications to generate customised quantum light states and required modifications to generate them.

[1] Fischer, K., Hanschke, et al. Signatures of two-photon pulses from a quantum two-level system. Nature Phys 13, 649-654 (2017).

HL 29.68 Tue 18:00 P1

Investigating Photo-Physical Properties of Ag-In-S Core and Core-shell Quantum Dots — •Johannes Kunze, Julian Mann, Sushant Ghimire, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

Non-toxic I-III-VI quantum dots (QDs) are promising candidates for next-generation light-emitting and energy-harvesting devices. However, the optical properties in these QDs are governed by subgap defects which limit their applications. Here, we synthesize AgInS2 QDs, and study them using various steady-state and time-resolved spectroscopy. Photoluminescence spectroscopy reveals that these QDs exhibit a narrow free-exciton emission and a more dominant, broad, red-shifted emission. The observed dominance arises from defects in the QDs, which introduce donor and acceptor states within the bandgap, effectively trapping electrons and holes from the band edge. A femtosecond differential transmission spectroscopy reveals an ultrafast carrier trapping time in these QDs. Additionally, a broad absorption onset with a defect-related Urbach tail is observed. We coated AgInS2 QDs with gallium sulfide, forming core/shell QDs, which significantly enhanced the intensity of the narrow free-exciton emission, reduced defect emissions, and sharpened the absorption onset by lowering the Urbach energy. These results show that the defects in these QDs are located on their surface, and Ga-S coating effectively passivates them, improving the excitonic characteristics.

HL 29.69 Tue 18:00 P1

Effects of vacancies in a bilayer graphene quantum dot — •Ivan Verstraeten, Robin Smeyers, François Peeters, and Lucian Covaci — University of Antwerp, Antwerp, Belgium

Confining the motion of an electron to the nanoscale in all three dimensions, i.e. a quantum dot (QD), sees the emergence of interesting physics and useful applications, such as single electron control or qubits. Bilayer graphene in particular, is a suitable and promising material for quantum dots owing to the many exotic properties of graphene, as well as the possibility to create and tune electronic confinement simply by applying a (position dependent) perpendicular electric field. In this work, the electronic spectrum of an electrostatically defined QD in a finite bilayer graphene flake is numerically calculated

using the tight-binding model, which is compared to existing results in the literature where a low-energy continuum theory was used. The tight-binding approach allows for a straightforward implementation of vacancies in the lattice, of which the effects on the spectrum and its valley character are studied. The results show a generally good agreement between the continuum and tight-binding theory, with some interesting discrepancies. We find that vacancies enhance the inter-valley scattering, as in the magnetic field dependence of the spectrum we observe a widening of the avoided crossings between energy levels of a different valley character. Furthermore, vacancies are found to be able to significantly shift energy levels, alter the shape of the wavefunction density and make a state retain its valley mixed character even in the presence of perpendicular magnetic field

HL 29.70 Tue 18:00 P1

Towards scalable quantum circuits based on microlaser-pumped quantum emitters — •Maximilian Klonz, Aris Koulas-Simos, Léo Roche, Imad Limame, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We report on activities towards the development of a scalable technology platform for integrated quantum photonic circuits (IQPCs) based on semiconductor quantum dots, which are deterministically integrated into photonic waveguides by in-situ electron beam lithography [1], acting as single-photon emitters. Photons, generated by these on-demand quantum emitters, serve as flying qubits in quantum communication systems and as input states for photonic quantum computing [2, 3]. Here, we present innovative technological approaches for a two-step epitaxial growth method to achieve areas with low and high density of quantum dots to further fabricate lasers and single-photon sources monolithically integrated on the same wafer. We show simulations towards a scheme for optical on-chip pumping of these single-photon emitters and first experimental results.

References
[1] P. Schnauber et al., Nano Letters 18, 2336 (2019)
[2] T. Heindel et al., Advances in Optics and Photonics 15, 613 (2023)
[3] S. Rodt and S. Reitzenstein., APL Photonics 6, 010901 (2021)

HL 29.71 Tue 18:00 P1

Duration of scattering processes on curved quantum wires — •Adrian Henrik Starke, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik

Over the last decade, the duration of quantum processes has become experimentally accessible via measurement of e.g. the Wigner time delay [1]. However, these measurements have so far only been performed in flat space. This study extends the concept of scattering time to curved, one-dimensional quantum wires. Wigner time delay and other parameters are examined for plane waves as well as wave packets constraint to propagate through these structures. The results demonstrate that the geometry-induced potentials significantly affect the scattering time, particularly at low energies, with the classical behavior emerging at higher energies. These findings offer insights into the interplay between curvature and quantum dynamics, paving the way for further analysis of scattering phenomena in complex geometries.

[1] Schulze et al., 'Delay in Photoemission'. In: Science 328 (2010), DOI: 10.1126/science.1189401

HL 29.72 Tue 18:00 P1

Towards a Quantitative Framework for Capacitance-Voltage Spectroscopy in Quantum Dot Ensembles — •Phil Julien Badura[1], Nico Frédéric Brosda[1], Ismail Bölükbaşı[1], Ibrahim Engin[1], Patrick Lindner[1], Sascha René Valentin[1], Andreas Dirk Wieck[1], Björn Sothmann[2], and Arne Ludwig[1] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47048 Duisburg, Germany

This study investigates an inhomogeneous ensemble of quantum dots coupled to a charge reservoir using capacitance-voltage spectroscopy. Experimental measurements reveal shifts in capacitance peak positions influenced by AC frequency and temperature, with frequency-dependent shifts remaining unexplained by existing models. To address this, we develop a master equation-based theoretical model incorporating energy-dependent tunneling effects, which successfully reproduces the experimental data. Our findings emphasize the role of energy-dependent tunneling in distinct regimes: at low temperatures, energy level dispersion dominates, while at high temperatures and frequencies, shifts arise from optimized sequences of in- and out-tunneling events.

HL 29.73 Tue 18:00 P1

Experimental time-bin encoding quantum key distribution with telecom semiconductor quantum dot — •Jipeng Wang[1], Jingzhong Yang[1], Joscha Hanel[1], Zenghui Jiang[1], Vincent Rehlinger[1], Raphael Joos[2], Stephanie Bauer[2], Sascha Kolatschek[2], Eddy Rugeramigabo[1], Michael Jetter[2], Simone Portalupi[2], Michael Zopf[1,3], Peter Michler[2], and Fei Ding[1,3] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany. — [3]Laboratorium für Nano-und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Quantum Key Distribution (QKD) enables secure data transmission via quantum-generated secret keys. Semiconductor quantum dots (QDs) are promising light sources for high-speed quantum networks due to their deterministic single-photon emission. However, polarisation stability in fibre networks is often disrupted by environmental factors. Here, we demonstrate a stable QKD scheme using time-bin qubits derived from polarised photons emitted by a QD in the telecommunication C-band. A 16-bit pseudo-random sequence is encoded via a Sagnac-loop interferometer and decoded using an unbalanced Mach-Zehnder interferometer after transmission through 80 km of fibre. This study highlights QDs' potential for scalable, robust quantum networks.

HL 29.74 Tue 18:00 P1

Experimental time-bin encoding quantum key distribution with telecom semiconductor quantum dot — •Jipeng Wang[1], Jingzhong Yang[1], Joscha Hanel[1], Zenghui Jiang[1], Vincent Rehlinger[1], Raphael Joos[2], Stephanie Bauer[2], Sascha Kolatschek[2], Eddy Rugeramigabo[1], Michael Jetter[2], Simone Portalupi[2], Michael Zopf[1,3], Peter Michler[2], and Fei Ding[1,3] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany. — [3]Laboratorium für Nano-und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

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HL 29.75 Tue 18:00 P1

Cyclic Growth of InAs Quantum Dots: Exploring Structure-Property Relations for Telecom O-Band Applications — •Lennart Anderson[1,2], Danial Kohminaei[1], Severin Krüger[1,3], Marcel Schmidt[1], Nikolai Spitzer[1], Peter Zajac[1,4], Andreas Wieck[1], and Arne Ludwig[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]ICAMS, Ruhr-Universität Bochum — [3]Sparrow Quantum ApS, Copenhagen — [4]Gesellschaft für Gerätebau mbH, Dortmund

Quantum dots (QDs) are promising single-photon emitters that could transform long-range quantum communication within telecom optical fiber transparency windows. In this study, we grow self-assembled InAs QDs using the Stranski-Krastanov growth mode, enhanced by a strain reduction layer to achieve emission at 1.3 μm in the telecom O-band. By employing cyclic sub-monolayer deposition, we observe periodic modulations in QD density, emission wavelength, and geometric properties, driven by nucleation waves, i.e. a new generation of QDs is formed each time a critical material amount for nucleation is reached. We explore the correlations between the structural characteristics and opto-electronic properties by atomic force microscopy and

photoluminescence as well as capacitance-voltage spectroscopy. Our results identify optimal regions for QD density and emission wavelength across 3-inch wafers and propose a modified deposition scheme to enhance the usable area of the wafers.

HL 29.76 Tue 18:00 P1

Statistical spectroscopy of perovskite quantum dots — •Christopher Borchers[1], Frederik Benthin[1], Tom Rakow[1], Pengji Li[1], Maximilian Heller[1], Chenglian Zhu[2,3], Ihor Cherniukh[2,3], Gabriele Rainò[2,3], Maksym Kovalenko[2,3], Michael Zopf[1,4], and Fei Ding[1,4] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics, Empa - Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland — [4]Laboratory of Nano and Quantum Engineering, Leibniz University Hannover, Schneiderberg 39, D-30167 Hannover, Germany

The ability to perform fast and automated photoluminescence (PL) spectroscopy measurements greatly improves the efficient development of quantum light emitters and their optimization in quantum technologies.

We adopt and semi-automate standard low temperature optical characterization measurements for lead halide perovskite colloidal quantum dots. Here, PL spectroscopy on CsPbBr3 samples is used to characterize the emission spectrum, polarization properties, and fine structure, and to perform corresponding automated statistical analyses of these measurements. For these analyses, we have developed a program that processes PL spectral data, automatically detecting and fitting emission peaks for subsequent evaluation.

HL 29.77 Tue 18:00 P1

SUPER drived quantum dot at telecom wavelength — •Zenghui Jiang[1], Vikas Remesh[2], Frederik Benthin[1], Michael Zopf[1], and Fei Ding[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Department of Experimental Physics University of Innsbruck Technikerstr. 25d, Office 01/503 6020 Innsbruck, Austria

To obtain the best photon properties from quantum dots (QDs),a direct drive between the S-shell and ground state (resonance excitation) is required. However, since the excitation laser and the emitted wavelength are very close to each other, filtering out the laser becomes highly challenging. A theoretical study conducted in 2021 by Prof. Doris Reiter's group predicted that with two relatively detuned laser pulses, full population inversion can still be achieved without interacting with other energy levels. Consequently, photon properties comparable to those achieved through resonance excitation can be expected.

To efficiently drive QDs, two temporally overlapping laser pulses with different frequencies are needed. Compared to using two separate lasers for "SUPER" excitation, employing a single laser with a pulse shaper eliminates the need for synchronization between two lasers. However, until now, no experiment using a single laser with a pulse shaper has been performed on telecom-wavelength QDs. In our work, we constructed a pulse shaper using a spatial light modulator to generate two sharply defined laser pulses from a single broadband laser pulse,and successfully *SUPER* excited QD at telecom wavelength.

HL 29.78 Tue 18:00 P1

Fabrication of Ohmic contact for Electrical tuning of GaAs quantum dots — •Krupali Dobariya[1], Tom Fandrich[1], Yiteng Zhang[1], Johann Dzeik[1], Arijit Chakraborty[1], Tom Rakow[1], Sulabh Shrestha[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover, Institut for Solid State Physics, Hannover, Germany — [2]Leibniz Universität Hannover, Laboratorium for Nano and Quantum Engineering, Hannover, Germany

Semiconductor quantum dots have shown unique properties as deterministic single photon and entangled photon pair sources. Their outstanding optical properties have the potential for use in quantum applications like quantum communication, quantum key distribution and quantum computing. Nevertheless, due to the stochastic nature of the self-assembly growth process, quantum dots typically emit photons with a broad wavelength distribution across the entire chip, posing challenges for applications requiring specific wavelengths. To address this issue, various tuning techniques have been developed. Electrical tuning, in particular, has emerged as an effective method for adjusting the wavelength and mitigating charge noise in semiconductor quantum dots. Our research focuses on the impact of contact fabrication on the emission properties of GaAs quantum dots. We aim to optimize the process of forming ohmic contacts to n- and p-doped GaAs, placing special emphasis on the selection of materials and the reduction of contact resistance. The quality and performance of the electrical contacts are evaluated through the photoluminescence characterization.

HL 29.79 Tue 18:00 P1

Marker-based deterministic EBL integration of GaAs quantum dots (QDs) into electrically tunable Circular Bragg Gratings (eCBGs) at a wavelength of 780 nm — •Dinara Basharova[1], Mudi Priyabrata[1], Avijit Barua[1], Setthanat Wijitpatima[1], Andreas D. Wieck[2], Sven Rodt[1], Arne Ludwig[2], Richard Warburton[3], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, DE-44780 Bochum, Germany — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Integration of high-quality quantum emitters with photonic structures is essential for advancing quantum information technologies. We present a marker-based deterministic electron beam lithography (EBL) technique to integrate Gallium Arsenide (GaAs) quantum dots (QDs) into electrically contacted Circular Bragg Gratings (eCBGs) at an emission wavelength of 780 nm, combined with a PIN-diode structure. eCBG devices not only enhance the photon extraction efficiency through a circularly symmetric cavity design but also provide precise electrical control over the QD emission. This enables fine-tuning of the wavelength, addressing spectral mismatches, and stabilizing the charge environment around the QD, critical for high-performance quantum light sources. Therefore, combining the eCBG design with deterministic fabrication techniques ensures that the QDs are precisely positioned at the cavity center, maximizing light-matter interaction.

HL 29.80 Tue 18:00 P1

Laboratory management software: Plexy : Python Library for EXperimental Physics — •Frederik Benthin, Christopher Borchers, Nico Eggeling, Tom Fandrich, Dolores García de Viedma, Joscha Hanel, Maximilian Heller, Martin Hesse, Kai Hühn, Johannes Knollmann, Marcel Pölking, Tom Rakow, Eduard Sauter, Pavel Sterin, Fei Ding, Jens Hübner, and Michael Zopf — Leibniz Universität Hannover, Institute of Solid-State Physics, Appelstraße 2, 30167 Hannover

Measurements often involve complex protocols requiring the coordination of many different devices. Laboratory management or measurement software such as Qudi and NOMAD-CAMELS assist in performing these tasks. It provides a framework for easier collaboration and sharing of resources. It often includes a standalone graphical user interface (GUI). This GUI controls new compound instruments consisting of several devices and can be used to coordinate the measurement. Different projects often improve an additional aspect, such as NOMAD-CAMELS with metadata collection or MAHOS with messaging between distributed devices. Here we present Python Library for EXperimental Physics (Plexy), which is a highly modular repository of Python modules. Among the main design goals are automatic metadata recording, distributed device coordination, modular and flexible but standardized code organization as well as independent and common GUIs. An analyzer GUI performs common analyses specific to photoluminescence spectroscopy and time-correlated single-photon counting of quantum dot single-photon sources.

HL 29.81 Tue 18:00 P1

Signatures of the quantum skyrmion Hall effect in the Bernevig-Hughes-Zhang model — •Reyhan Ay, Adipta Pal, and Ashley M. Cook — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Given the recent discovery of the quantum skyrmion Hall effect (QSkHE) revealing that the 2+1 D SU(2) gauge theory should be generalized to include terms from an underlying 4+1 D SU(2) gauge theory subjected to generalized fuzzification, we re-examine the canonical Bernevig-Hughes-Zhang (BHZ) model for the quantum spin Hall insulator (QSHI). Considering that the isospin degrees of freedom in the tight-binding model Hamiltonian effectively encode two additional spatial dimensions, we identify signatures of topological states within the QSkHE framework related to intrinsically 4+1 D topological phases revealed by breaking time-reversal symmetry through a weak Zeeman

field. We identify distinctive real-space boundary orbital angular momentum textures due to the QSkHE, as well as gapless boundary modes that are robust against magnetic disorder, which is unexpected for a QSHI but predictable for compactified boundary 3D Weyl nodes in a topological skyrmion phase. Revisiting experimental work on robust edge conduction in HgTe quantum wells under Zeeman and orbital magnetic fields, we find these results consistent with theoretical predictions of compactified boundary 3D Weyl nodes to such external fields. These experiments are thus potentially the first-known experimental observation of the quantum skyrmion Hall effect.

HL 29.82 Tue 18:00 P1

Side-contacted narrow superconducting finger on quantum anomalous Hall insulator — •Bibek Bhujel, Anjana Uday, Gertjan Lippertz, Alexey A. Taskin, and Yoichi Ando — Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany

Recently, the evidence for superconducting pair correlation is obtained in the chiral edge states of a vanadium-doped $(Bi_xSb_{1-x})_2Te_3$ thin film, tuned to the quantum anomalous Hall insulator phase by observing the negative nonlocal resistance downstream from a narrow superconducting (grounded) Nb finger electrode fabricated on the top [1]. This negative downstream resistance is due to the crossed Andreev reflection (CAR) process, which creates superconducting correlations in the chiral edge. To investigate this observation further, we are currently fabricating side-contacted Al and Nb finger electrodes on the etched QAHI. One of the main advantages of fabricating the side-contacted electrodes is their low contact resistance, which has high reproducibility. We will report on our progress on this project so far.

[1] Uday, A., Lippertz, G., Moors, K. et al. Induced superconducting correlations in a quantum anomalous Hall insulator. Nat. Phys. 20, 1589*1595 (2024). https://doi.org/10.1038/s41567-024-02574-1

HL 29.83 Tue 18:00 P1

Anomalous Hall effect in a two-dimensional disordered Lorentz gas — •Frederik Bartels[1], Zakaria Harroud[1], Beate Horn-Cosfeld[1], Mihai Cerchez[1], Jürgen Horbach[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Theoretical Physics II: Soft Matter, Heinrich Heine University, Düsseldorf, Germany

Using a combination of experiment and simulation, it was studied the magnetotransport in a two-dimensional disordered Lorentz gas with cross-shaped obstacles. Our focus is on the investigation of the Hall effect for obstacle densities beyond the low-density limit. From previous studies, we know that for lower obstacle densities, the magnetotransport properties, as obtained from the simulation and the experiment of a pristine sample, can be well described in terms of the Drude-Boltzmann model. At higher obstacle densities, deviations from the normal Hall effect are observed, depending on both obstacle density and magnetic field. These results extend previous studies on circular obstacles, where similar deviations were observed and the Hall coefficient does not accurately reflect the electron density because of the presence of memory effects. [1]

[1] B. Sanvee *et al.* Phys. Rev. B **108**, 035301 (2023)

HL 29.84 Tue 18:00 P1

Accelerated Electrical Transport Predictions of the Non-Perturbative ab initio Kubo-Greenwood Method via a Deep-learned Hamiltonian technique: Strongly Anharmonic Material Cases — •Juan Zhang, Jingkai Quan, Matthias Scheffler, and Kisung Kang — The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany

High-performance thermoelectric materials are characterized by low thermal and high electrical conductivities. Thermal insulators with ultra-low thermal conductivity feature strong anharmonicity, also significantly affecting electronic transport [1]. Strong anharmonicity impedes the application of perturbative methods due to the breakdown of the quasi-particle picture. This challenge can be overcome by the non-perturbative ab initio Kubo-Greenwood approach (aiKG)[1]. However, the aiKG method requires substantial computational cost due to its extensive supercell electronic structure evaluations at each step during ab initio Molecular Dynamics (aiMD). A recent deep neural network technique to train and predict the Kohn-Sham Hamiltonian, implemented by DeepH[2], can provide an efficient bypass to extract the electronic structure of each MD step with nearing ab initio accuracy. This work introduces an AI-assisted aiKG formalism with accelerated carrier mobility evaluations, exemplified by its application to strongly anharmonic materials. We thoroughly examine DeepH's capability for electronic property predictions with its spatial scalability.

[1] J. Quan et al., Phys. Rev. B, accepted (arXiv:2408.12908).
[2] X. Gong, et al., Nat Commun. 14, 2848 (2023).

HL 29.85 Tue 18:00 P1

Magnetotransport in the correlated metal $CaVO_3$ — •Olivio Chiatti[1], Mahni Müller[1], Maria Espinosa[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and Saskia F. Fischer[1,4] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Transparent conductive materials are in great demand in the optoelectronic industry for their high-performance and cost-effectiveness. Enhancing the carrier effective mass through strong electron-electron interactions in correlated metals is a promising approach to achieve both high-optical transparency and high-electrical conductivity [1]. Here, we study the electric transport properties of thin $CaVO_3$ films grown on $LaAlO_3$ substrates by hybrid molecular beam epitaxy, with residual resistivity ratio (RRR) up to 98 [2]. Magnetoresistance and Hall measurements were performed between 50 mK and 300 K. Films with high RRR show nonlinear Hall resistivities and linear magnetoresistance below 40 K. Shubnikov-de Haas oscillations are also observed for magnetic fields above 6 T. The application of a multi-carrier model and the complex Fermi surface of $CaVO_3$ are discussed.

[1] Zhang *et al.*, Nature Materials **15**, 204 (2016)
[2] Kuznetsova *et al.*, APL Materials **11**, 041120 (2023)

HL 29.86 Tue 18:00 P1

Selenium, Silicon and SiC power diodes as temperature sensors, operated in different voltage regimes and under extreme conditions — •Heinz-Christoph Neitzert, Arpana Singh, and Vincenzo Carrano — Dept. of Industrial Engineering (DIIn), Salerno University, Via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy

Commercial semiconductor temperature sensors are nowadays mostly based on silicon diodes and transistors, operated under constant forward current conditions. We compared the temperature sensing capabilities of a series of different power diodes from different materials not only in the forward, but also in the reverse bias and in one example also in the breakdown voltage regime. All investigated devices, including the historical Se rectifiers, showed stable temperature sensing capabilities in the forward bias regime under moderate temperature changes. Some of them have been tested under extreme conditions like extreme temperatures and particle irradiation. In particular it is shown in the case of the SiC Schottky diodes, that the excellent temperature sensing properties are also maintained after irradiation with high energy ions. In the case of Silicon pn diodes the sensitivity as sensor in the forward voltage and avalanche breakdown regime has been determined. In both regimes the sensors showed very good linear characteristics, when biased under constant current conditions. For Silicon diodes, also the temperature limit, where no irreversible device changes are observed has been determined and the defect creation for higher temperatures has been monitored.

HL 29.87 Tue 18:00 P1

Structural Dynamics of Excimer Formation in single crystalline α-Perylene — •Helena Hollstein[1], Simon Versmissen[2], Bram Spijkerman[2], Heinrich Schwoerer[2], and Sebastian Hammer[1] — [1]University of Würzburg, 97074 Würzburg, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany

In the field of organic semiconductors an exact understanding of the formation of multi-molecular excited states, such as excimers, and geometric inter-molecular changes caused thereby, is crucial but challenging. Quantum chemical methods are in principle able to capture all structural changes during excimer formation but are hardly feasible due to the complexity of organic crystals. Experimentally on the other hand, the molecular motion can be detected by ultra-fast electron diffraction (UED) on a femtosecond timescale [1], and by using structural modeling the molecular movement can be reconstructed from changes in the diffraction pattern [2].

In this contribution we examine the structural reorganization during the formation of the low lying excimer state in single crystalline

perylene in its crystallographic α-phase by means of UED. We are able to reveal the pathways of the geometric relaxation during the excimer formation on a fs timescale and find that the formation happens on a 5 ps timescale.

HL 29.88 Tue 18:00 P1

All-optical spin injection in silicon investigated by element-specific time-resolved Kerr effect — Simone Laterza[1,2], Antonio Caretta[1], •Richa Bhardwaj[1,3], Roberto Flammini[4], Paolo Moras[5], Matteo Jugovac[5], Piu Rajak[6], Mahabul Islam[6], Regina Ciancio[6], Valentina Bonanni[1], Barbara Casarin[2], Alberto Simoncig[1], Marco Zangrando[1,6], Primož R. Ribič[1], Giuseppe Penco[1], Giovanni De Ninno[1], Luca Giannessi[1], Alexander Demidovich[1], Miltcho Danailov[1], Fulvio Parmigiani[1], and Marco Malvestuto[1,6] — [1]Elettra Sincrotrone Trieste, Italy — [2]University of Trieste, Italy — [3]Institute of Physics and Center for Nanotechnology (CeNTech), University of Münster, 48149 Münster, Germany — [4]Istituto di Struttura della Materia-CNR (ISM-CNR), Roma, Italy — [5]Istituto di Struttura della Materia-CNR (ISM-CNR), Trieste, Italy — [6]Istituto Officina dei Materiali (CNR-IOM), Trieste, Italy

Understanding how a spin current flows across metal-semiconductor interfaces at pico- and femtosecond time scales is of paramount importance for ultrafast spintronics, storage applications etc. However, the possibility to directly access the propagation of spin currents, within such time scales, has been hampered by the simultaneous lack of both ultrafast element-specific magnetic sensitive probes and tailored well-built and characterized metal-semiconductor interfaces. Here, by means of a novel free-electron laser-based element-sensitive ultrafast time-resolved Kerr spectroscopy, we reveal different magnetodynamics for the Ni $M_{2,3}$ and Si $L_{2,3}$ absorption edges.

HL 29.89 Tue 18:00 P1

Implementation and operation of a fiber-coupled CMOS detector for time-resolved photoemission electron microscopy — •Philipp Kessler[1], Johanna Kinder[1], Victor Lisinetskii[1], Torsten Franz[2], Florian Schütz[2], Matthias Hensen[1], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]ELMITEC Elektronenmikroskopie GmbH, 38678 Clausthal-Zellerfeld

Since their invention, low-energy electron microscopy (LEEM) and photoemission electron microscopy (PEEM) have predominantly relied on microchannel plates for electron detection and image generation. Recent developments in detector technology allow the LEEM-PEEM community to use pixel- [1] and fiber-based [2] detectors that have a small detection pixel size, avoid blooming effects, and have an extended dynamic range. These advancements are particularly beneficial for ultrafast time-resolved experiments with weak signals. Here, we present the integration of the fiber-coupled CMOS detector XF416 (TVIPS GmbH, Germany) into an Elmitec AC-LEEM III system. This includes a structural solution to address the detector's inability to undergo bake-out, a critical step for achieving ultrahigh vacuum conditions. The first-time operation of the new detector unit is demonstrated through time- and energy-resolved PEEM measurements on terrylene bisimide-based molecular thin films, enabling the study of exciton dynamics at the nanoscale.

[1] G. Tinti et al., J. Synchrotron Rad. 24, 963 (2017).
[2] D. Janoschka et al., Ultramicroscopy 221, 113180 (2021).

HL 29.90 Tue 18:00 P1

Experimental scheme for high-order fluorescence-detected pump–probe micro-spectroscopy on monolayer MoS_2 — •Ruidan Zhu, Patrick Grenzer, Simon Büttner, Matthias Hensen, Tobias Hertel, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Monolayers of transition metal dichalcogenides (TMDCs) are two-dimensional (2D) semiconductors with fascinating optoelectronic properties. However, exciton–exciton interaction (EEI) sets a fundamental limit to optimizing the quantum efficiency of 2D materials under high exciton densities. In particular, EEI processes are frequently mixed with single-exciton dynamics, thereby complicating the elucidation of their underlying mechanisms. Here, we apply fluorescence-detected pump–probe spectroscopy [1] in a cryomicroscope to detect the exciton dynamics of monolayer MoS_2. By incorporating the high-order separation methods that we recently developed [2], we aim to isolate EEI dynamics from the single-exciton dynamics, other higher-order signal contributions, and non-resonant substrate responses. We present the fundamental concept, the experimental setup, and the first data.

[1] P. Malý and T. Brixner, Angew. Chem. Int. Ed. 2021, 60, 18867.
[2] P. Malý et al., Nature 2023, 616, 280.

HL 29.91 Tue 18:00 P1

Detection Strategies for Highspeed Impulsive Stimulated Raman Scattering — •Laura Hüllmandel, Julia Lang, and Georg Herink — Universität Bayreuth

Impulsive stimulated Raman scattering is an established method for resolving transient coherent superpositions of optical phonons in matter. Inside a laser cavity, however, this nonlinear interaction between multiple ultrashort temporal solitons can accumulate and determine their trajectories [1]. In this contribution, we study different regimes of the coupling between solitons via optical phonons. Based on extra-cavity spectroscopic experiments on crystalline media, we compare interferometric and spectrally-resolved sampling modes and, in particular, we discuss practical aspects in enhancing Raman signal quality. These new insights contribute to the understanding of phonon-driven soliton coupling and the development of time-domain intra-cavity Raman spectroscopy.

[1] A. Völkel et al., "Intracavity Raman Scattering Couples Soliton Molecules with Terahertz Phonons.", Nature Communications 13.1 (2022).

HL 29.92 Tue 18:00 P1

Two-dimensional spectroscopy setup for the investigation of excitons and polaritons in 2D materials — •Trideep Kawde, Pavel Trofimov, Matteo Russo, Anton Trenczek, David Koch, and Hélène Seiler — Freie Universität Berlin, 14195, Berlin, Germany

Coherent two-dimensional (2D) electronic spectroscopy is a powerful tool for probing interactions between electronically excited states and map their evolution in both energy and time domains. Here we introduce a coherent two-dimensional spectrometer tunable over the 460-950 nm spectral range to investigate the exciton and polariton dynamics in 2D materials. We employ a hollow-core fiber setup for broadband visible continuum generation. Pulse shapers are used to produce phase-locked sequences of pulses. A custom sample area has been designed specifically for 2D materials, typically featuring high degrees of spatial inhomogeneity and small sizes (few tens of micrometers). Linear spectroscopies can be performed at the same position as the 2D spectroscopy experiments, including angle-resolved spectroscopy to investigate polariton dispersion. With our setup we will be able to reveal insights into excitonic and polaritonic properties in 2D materials.

HL 29.93 Tue 18:00 P1

Measurement of ultrashort electron pulse durations using a transient electric field — •Lukas Nöding, Arne Ungeheuer, Ahmed Hassanien, Mashood Tariq Mir, Thomas Baumert, and Arne Senftleben — University of Kassel, Institute of Physics, Kassel, Germany

Ultrafast electron diffraction is a well-known method for conducting time-resolved measurements on molecules and condensed matter. In this approach, electron diffraction is performed with an electron pulse at a variable time after optical excitation of the sample. The duration of the electron pulse directly determines the temporal resolution. A streaking setup utilizing free electrons is implemented to measure the duration of the electron pulse. Therefore, a transient electron deflector, was designed. Its main feature is a metal surface parallel to the path of the electron pulse. A femtosecond laser pulse is focused from the side onto this metal surface. As the beam incides, electrons are released from the metal. Due to their momentum, they separate from the surface, create an electric field perpendicular to the surface and then recombine. The build-up and the subsequent fading of this transient electric field is used to streak the electron pulse, because different electrons in the pulse experience different field strengths. By that, the duration of the pulse is mapped into a spatial broadening of the pulse. The broadening is captured by the detector as a streak. We will show results measured with different numbers of electrons per pulse and compare them with simulations. Moreover, the evaluation process and the fitting algorithms for the electron streak will be explained.

HL 29.94 Tue 18:00 P1

Ultrafast dynamics reveal proximity induced changes in Graphite — •Mashood Tariq Mir, Ahmed Hassanien, Arne

Ungeheuer, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics, D-34132 Kassel, Germany

Layered transition metal dichalcogenides (TMDs) are at the forefront of materials research due to their diverse electronic and structural properties. Among these materials, 1T-TaS2 exhibits a complex temperature-dependent phase diagram characterized by charge density waves (CDWs) of varying commensurabilities. When integrated into heterostructures, novel interfacial phenomena emerge, enabling the study of proximity effects in atomically thin materials. This work investigates the light-induced dynamics of a van der Waals heterostructure composed of 1T-TaS2 and graphene using ultrafast electron diffraction (UED). Femtosecond laser pulses induce rapid structural changes, revealing a proximity-induced CDW in graphene. This observation demonstrates how interfacial coupling can imprint the characteristic periodic lattice modulation of CDWs onto an otherwise non-CDW material. By controlling lattice heating, we probe the reversible phase transition of 1T-TaS2 from the nearly commensurate to the incommensurate phase and its influence on the interfacial properties of the heterostructure.

HL 29.95 Tue 18:00 P1

Determination of Arrival Time in Ultrafast Electron Diffraction in Specimen Close Proximity with High Accuracy — •Ahmed Hassanien, Mashood Tariq Mir, Arne Ungeheuer, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

The ability to determine time zero in a pump-probe experiment qualitatively indicates its ability to capture dynamics and quantitatively serves as a measure of its temporal resolution. There are only a few methods for determining the time zero in ultrafast electron diffraction (UED) [1,2]. Here, we propose a robust and easy-to-implement method to determine time zero in the immediate vicinity of the sample with sub-picosecond accuracy using Fourier-transformed electron micrography (FT-EM). In the same analogy as the Debye-Weller effect in crystalline solids, the attenuation of the peak amplitude in FT-EM patterns for a metal grid blurred by femtosecond optically-induced transient electrostatic lensing (TEL) allowed us to determine time zero to better than 500 fs. To demonstrate our method, we measured the time zero in the vicinity of a graphite flake, for which we also performed a routine UED measurement by exciting with the same optical pump fluence, well below the damage threshold for either material. Using the accurately determined time zero, we were able to identify the earlier onset of the out-of-plane coherent optical phonon mode in graphite. References: [1] Olshin, Pavel K., et al. APL 120.10 (2022). [2] Dwyer, Jason R., et al. Philos. Trans. of the Royal Society A: Math., Phys. and Eng. Sci. 364.1840 (2006): 741-778.

HL 29.96 Tue 18:00 P1

Investigation of dynamics and character of excitons in WSe_2 multilayers — •Anna Weindl[1], Matthias Brem[1], Jennifer Lehner[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan

We report about our time-resolved Faraday ellipticity (TRFE) experiments on multilayers of the transition metal dichalcogenide WSe_2. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the temporal dynamics in WSe2 multilayers. These previous results have shown that pseudospin oscillations appear in the TRFE signal when we apply an in-plane magnetic field to our multilayer samples. Current results show that the oscillations have two different frequencies, a shorter one earlier in time and a longer one later in time. In differential transmission measurements, the lifetimes show a fast and slow decay on the same time scales. This suggests two different exciton dynamics or species. Now we try to characterize and manipulate these oscillations by playing with different experimental parameters. Varying the angle of the magnetic field, adding an electric field or investigating the layer dependence are examples for our toolbox of parameters to gain further insights in the dynamics of the multilayers. [1] Raiber et al., Nat Commun 13, 4997 (2022).

HL 30: Focus Session: Young Semiconductor Forum

The young semiconductor forum gives a platform for post-docs at all career stages to present themselves and their scientific ideas. It consists of an oral session with invited talks and immediately afterwards, a poster session, where further participants present a poster about their work and/or scientific vita. With this format, we hope to attract both postdocs and senior researchers and decision makers to join this forum: for postdocs, to give them a platform to present themselves, and for professors, to meet the next generation of scientists.

Organized by Alexander Holleitner and the AGyouLeaP (Susanne Liese, Alexander Schlaich, and Christoph Kastl)

Time: Wednesday 9:30–12:15 Location: H13

Invited Talk HL 30.1 Wed 9:30 H13

Exploring semiconducting epigraphene grown by polymer-assisted sublimation growth — •Teresa Tschirner, Julia Guse, Stefan Wundrack, Frank Hohls, Klaus Pierz, and Hans Werner Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Epitaxial graphene on SiC is a potential candidate in a variety of applications, such as the fabrication of 2D heterostructures and the intercalation of graphene layers with other materials for engineering new electronic material systems. Important for the quality of the graphene is the 0th layer, or buffer layer, which is covalently bonded to the SiC substrate. The buffer layer itself can be functionalized by intercalation. In a recent study it was shown that an electronic bandgap can be opened in the otherwise gapless buffer layer. The semiconducting epigraphene (SEG) on SiC has a bandgap of 0.6 eV and high room temperature mobilities (5000 cm^2/Vs), much larger than silicon and other 2D-semiconductors [1]. In this study we grow high-quality buffer layers not only across single terraces as in the aforementioned study but on millimeter scale, due to an advanced growth technique preventing step bunching and large terrace step heights. We use a polymer-assisted sublimation growth (PASG) method, where pretreatment of the SiC substrate supplies additional carbon and stabilizes the SiC surface by rapid buffer layer-formation preventing step-bunching. We investigate the growth parameters for homogeneous buffer layer formation with our PASG method and systematically study its structural properties and characteristics. [1] J. Zhao et al., Nature 625, 60 (2024).

Invited Talk HL 30.2 Wed 10:00 H13

Huge Enhancement of the Giant Negative Magnetoresistance with Decreasing Electron Density — •Lina Bockhorn[1], Christian Reichl[2], Werner Wegscheider[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases often show a remarkably robust negative magnetoresistance at zero magnetic field. Below 800 mK, this phenomenon divides into two distinct parts [1-4]: a temperature-independent narrow peak around $B = 0$ T, arising from the interplay of smooth disorder and elastic scattering at macroscopic defects [2, 3], and a temperature-dependent giant negative magnetoresistance (GNMR) at higher magnetic fields. The theoretical understanding of the GNMR remains an open question, as it involves

several independent parameters in addition to electron-electron interaction possibly leading to hydrodynamic transport effects. To gain insights into the nature of the GNMR, we investigate this effect as a function of electron density at various temperatures and currents. Our results show a significant dependence of GNMR on electron density [4], indicating that variations in scattering potentials [5] are not considered appropriately in theoretical models. [1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011). [2] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014). [3] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016). [4] L. Bockhorn et al., Phys. Rev. B 109, 205416 (2024). [5] Y. Huang et al., Phys. Rev. Materials 6, L061001 (2022).

Invited Talk HL 30.3 Wed 10:30 H13

Ultrafast quantum optics with single-photon emitters in 2D materials — •Steffen Michaelis de Vasconcellos — Physikalisches Intitut, Universität Münster, Germany

Single-photon sources are essential components for building quantum networks, though achieving optimal control remains a significant challenge in advancing quantum technologies. Recently, 2D van der Waals materials, such as transition metal dichalcogenides (TMDs) and hexagonal boron nitride (hBN), have emerged as promising platforms for solid-state quantum light emitters, enabling new possibilities for creating, tuning, and integrating quantum emitters into photonic devices [1].

In my talk, I will review the development of single-photon emitters in 2D materials, focussing particularly on the robust emitters in hBN, which efficiently emit single photons even at room temperature. We demonstrate the efficient collection of single-photons by 3D-printed microlenses [2] and explore ultrafast coherent control of individual hBN quantum emitters [3]. Understanding the underlying dephasing mechanisms is key to designing devices that meet the requirements for future quantum technologies. Our work paves the way towards controlled hybrid quantum systems integrating electronic and phononic excitations.

[1] S. Michaelis de Vasconcellos, et al., Single-Photon Emitters in Layered Van der Waals Materials, phys. status solidi (b) 259, 2100566 (2022) [2] J. A. Preuß, et al., Nano Lett. 23, 407 (2023) [3] J. A. Preuß, et al., Optica 9, 522 (2022)

15 min. break

Invited Talk HL 30.4 Wed 11:15 H13

Realistic simulation of quantum emitter dynamics made easy — •Moritz Cygorek — TU Dortmund, Germany

Few-level quantum emitters such as quantum dots are a main workhorse for cutting edge research in quantum science, e.g., for nonclassical light generation. A practical challenge is the strong interaction with the physical environment such as phonons, which gives rise to a plethora of effects such as decoherence, phonon-assisted transitions, and renormalization. The intricacy of environment effects and computational challenges have in the past rendered the theoretical analysis an expert topic requiring an in-depth understanding of various theoretical methods.

Here, I demonstrate how the concept of process tensor matrix product operators (PT-MPOs) enables quick-and-easy, yet numerically exact simulations of very general open quantum systems. A computational framework is presented that can be used as a black box by the practitioner, which (i) requires no expert knowledge, (ii) leverages path integrals and tensor networks for exceptional speed and accuracy, (iii) is based on C++ for computational and memory efficiency, (iv) yet can be controlled by parameter files and requires no explicit programming, (iv) while also providing Python bindings for easy postprocessing.

Moreover, I demonstrate applications to solid-state cavity-QED relating to concrete experiments: single- and entangled photon generation, multitime correlation functions and dynamically dressed Mollow spectra, as well as phonon effects on cooperative emission and superradiance.

Invited Talk HL 30.5 Wed 11:45 H13

Data-driven Design of Next Generation 2D Materials and Their Heterostructures — •Rico Friedrich — TU Dresden — Helmholtz-Zentrum Dresden-Rossendorf — Duke University, USA

Two-dimensional (2D) materials and their heterostructures provide an extensive platform for realizing advanced electronic and magnetic functionalities at the nanoscale. While individual 2D systems are traditionally obtained from bulk layered compounds bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of semiconducting non-vdW 2D materials derived from non-layered crystals [1] opens up a new direction.

As outlined by our recent data-driven investigations employing autonomous *ab initio* calculations [2, 3], several dozens of new candidates showcase a wide range of appealing electronic, optical, and in particular magnetic properties owing to the (magnetic) cations at the active surfaces of the sheets. Further generalizing the data-driven modelling approach to all inorganic compounds provides fundamental insights into the exfoliation and cleavage of crystals. At the same time, chemical tuning by surface passivation provides a valuable handle to further control the electronic and magnetic properties of these next generation 2D compounds [4]. These features thus make non-vdW 2D materials an attractive platform for fundamental as well as applied nanoscience.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[4] T. Barnowsky *et al.*, Nano Lett. **24**, 3974 (2024).

HL 31: Focus Session: Young Semiconductor Forum Poster

The young semiconductor forum gives a platform for post-docs at all career stages to present themselves and their scientific ideas. It consists of an oral session with invited talks and immediately afterwards, a poster session, where further participants present a poster about their work and/or scientific vita. With this format, we hope to attract both postdocs and senior researchers and decision makers to join this forum: for postdocs, to give them a platform to present themselves, and for professors, to meet the next generation of scientists.

This part is the poster session.

Organized by Alexander Holleitner and the AGyouLeaP (Susanne Liese, Alexander Schlaich, and Christoph Kastl)

Time: Wednesday 12:15–13:00 Location: H13

HL 31.1 Wed 12:15 H13

Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, and Manfred Bayer — Experimentelle Physik 2a, TU Dortmund University, Dortmund, Germany

We demonstrate self-sustained auto-oscillations in a dissipative electron-nuclear spin system (ENSS) in semiconductors, where spontaneous breaking of translational symmetry in time produces robust limit-cycle dynamics across a broad range of parameters, including laser power, temperature, and magnetic field. These periodic oscillations exhibit coherence times extending to hours, reflecting ideal "time atom" ordering within the auto-oscillatory system.

Additionally, we uncover synchronization within excited subsystems without additional modulation, identifying its microscopic origins. Under periodic driving, modulation of parameters such as excitation power and pump polarization yields parametric resonances, signaling a transition to discrete auto-oscillatory behavior. Key phenomena include frequency entrainment, Arnold tongues, bifurcation jets, and a devil's staircase, showcasing the ENSS's versatility in exploring nonlinear dynamics, with broad implications for both fundamental physics

and semiconductor applications.

HL 31.2 Wed 12:15 H13

Reducing waste through substrate reuse: a pathway to cost-effective iii-v optoelectronics — •Radouane Ennadir — 3IT, Sherbrooke University, Sherbrooke, QC, Canada

III-V materials, such as Gallium Arsenide (GaAs), are widely used in optoelectronic devices due to their superior electronic and optical properties. However, the high cost of III-V substrates, primarily made from Ge or other expensive materials, represents a significant barrier to the widespread adoption of these technologies.

Our research focuses on reducing waste in the production of III-V optoelectronics through the reuse of Germanium (Ge) substrates. In this study, we propose a novel approach to mitigate substrate waste by reusing Ge substrates in the fabrication of III-V optoelectronics. By carefully optimizing the recycling process, including substrate cleaning, surface treatment, and the integration of new III-V layers, we aim to significantly reduce material costs without compromising device performance. This approach not only enhances the sustainability of optoelectronic manufacturing but also provides a cost-effective pathway to large-scale production of III-V-based devices. The findings of this study contribute to both environmental sustainability and economic viability in the growing field of optoelectronics, opening up new opportunities for the development of advanced, cost-effective optoelectronic devices.

HL 31.3 Wed 12:15 H13

1D exciton confinement in monolayer $MoSe_2$ near ferroelectric domain walls in periodically poled $LiNBo_3$ — •Pedro Soubelet, Yao Tong, Asier Astaburuaga Hernandez, Andreas V. Stier, and Jonathan J. Finley — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Monolayer transition metal dichalcogenides are an emergent platform for exploring and engineering quantum phenomena in condensed matter. Due to their atomic thickness, the excitonic response is highly influenced by the dielectric environment. In this work, we explore the optical properties and exciton kinetics of monolayer thick $MoSe_2$ straddling domain wall boundaries in ferroelectric periodically poled $LiNbO_3$ (PPLN). Spatially resolved photoluminescence (PL) experiments reveal sorting of neutral and charged excitons across the boundary. Our results reveal evidence for extremely large in-plane electric fields ($\simeq$4000 kV/cm) at the domain wall (DW), whose effect is manifested in the routing of free charges and trions towards oppositely poled domains, resulting in a nonintuitive spatial PL intensity pattern. In a second step, we engineer the PPLN substrate and the 2D heterostructure to exploit the non-uniform in-plane electric field exerted by the DW to confine neutral excitons in a 1D dipolar gas. Reducing the dimensionality holds an excellent potential for unlocking strong exciton-exciton interaction regimes, enabling exploration of exotic quantum phases of matter and designing advanced optoelectronic devices.

HL 31.4 Wed 12:15 H13

Probing strong electron-phonon coupling in graphene by resonance Raman spectroscopy with infrared excitation energy — •Simone Sotgiu[1,2], Tommaso Venanzi[1], Lorenzo Graziotto[1], Francesco Macheda[1], Taoufiq Quaj[2], Elena Stellino[1], Bernd Beschoten[2], Christoph Stampfer[2], Francesco Mauri[1], and Leonetta Baldassarre[1] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

Resonance Raman spectroscopy (RRS) has been a key asset to study the interplay between electronic and vibrational properties of graphene. We report on RRS measurements with an excitation photon energy down to 1.17 eV on mono (MLG) and bilayer (BLG) graphene, to study how low-energy carriers interact with lattice vibrations. Thanks to the excitation energy close to the Dirac point, we unveil in the MLG a giant increase of the intensity ratio between the double-resonant 2D and 2D* Raman peaks with respect to graphite [1]. In BLG, the low excitation energy hampers some of the resonant Raman processes giving rise to the 2D peak. Consequently, the subfeatures composing the 2D mode are spectrally more separated with respect to visible excitations. We compare experimental measurements on BLG with ab initio theoretical calculations and we trace back such modifications on the joint effects of probing the electronic dispersion close to the band splitting and enhancement of electron-phonon matrix elements [2]. [1] T. Venanzi et al., Phys. Rev. Lett. 2023, 130, 256901 [2] L. Graziotto et al., Nano Lett. 2024, 24, 1867

HL 31.5 Wed 12:15 H13

Effects of atomistic fluctuations on the excitonic fine-structure in alloyed colloidal quantum Dots — •Anne Nadine Tewonoue Djota, Surender Kumar, and Gabriel Bester — Institute of physical chemistry and physics, University of Hamburg

The electron-hole exchange interaction in the presence of spin-orbit coupling leads for an atomistic calculation to a small energy splitting of the excitonic state known in this context as the fine structure splitting (FSS). Although this splitting is typically small, it has large consequences for the optical properties. For instance, the photoluminescence originates from these few states and is governed by the splitting (giving rise to temperature dependence) and polarization of these low energy excitonic states. So far most of the theoretical modeling has assumed that high symmetry structures lead to a simple dark-bright splitting with a large degeneracy of the excitonic states. In this work, we show based on atomistic calculations, that even globally perfectly symmetric structures (i.e., as far as an atomistic construction permits a "spherical" quantum dot) show a qualitatively different FSS as soon as alloying is introduced. The alloying effect is significantly stronger than any global shape anisotropy where the symmetry is broken for instance by geometrical elongation of the quantum dot. On the other hand, alloying a quantum dot through processes such as cation exchange is inherently random. As a result, different random alloy configurations with the same size and composition can exhibit significantly different FSS.

HL 31.6 Wed 12:15 H13

Resistance standards from artifact wire coils to graphene quantum Hall resistance — •Yefei Yin[1], Mattias Kruskopf[1], Stephan Bauer[1], Teresa Tschirner[1], Klaus Pierz[1], Frank Hohls[1], Rolf J. Haug[2], and Hans W. Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Historically, resistance standards were made by physical artifact wire coils before 1990 and quantum resistors based on GaAs heterostructures after 1990. However, conventional GaAs quantum Hall resistance (QHR) standards with the quantized resistance $R_H = h/2e^2$ are operating under high magnetic flux densities B > 10 T, limited currents I < 50 μA, and low temperatures T < 1.5 K, which significantly hinder the dissemination of primary resistance standards. In this work, we developed practical primary QHR standards based on n- and p-type epitaxial graphene. This study first systematically demonstrated that p-type epitaxial graphene can also be used for primary resistance standards, as accurate (10^{-9} accuracy) as GaAs and n-type graphene counterparts for realizing the SI unit ohm in quantum metrology. [1] The n-type graphene QHR standards achieved the world best performance so far with a 10^{-9} accuracy under relaxed conditions (B = 4.5 T, I = 232.5 μA, T = 4.2 K) simultaneously. [2-3] Our graphene QHR standards have been utilized in the national metrology institutes in European countries. [1] Appl. Phys. Lett., 125, 064001 (2024). [2] Adv. Phys. Res. 1, 2200015 (2022). [3] Phys. Rev. Applied, 2024

HL 31.7 Wed 12:15 H13

Hybridized excitons in 2D van der Waals materials — •Andreas Stier — Walter Schottky Institut und TUM School of Natural Sciences, TU München, Garching, Deutschland

I will review our recent progress on magneto optical spectroscopy of atomically thin materials in magnetic fields up to 91 T with an emphasis on the spin-valley physics of neutral and charged excitons.

In monolayer (ML) semiconductors, magneto-absorption spectroscopy revealed the diamagnetic shifts of the exciton Rydberg states, which allowed the first direct experimental measure of the reduced mass and binding energy. Surprisingly, investigating the photoluminescence, we observe the emergence of a new excitonic peak, which we discuss in the framework of the theoretically predicted linear dispersing exciton branch originating from intervalley exchange interactions.

For heterostructures (HS) of a 2D semiconductor with graphene, we find a new multi-step proximity effect due to band folding in the HS, where we show that the spin-valley physics can be used to quantify interlayer hybridization. In HS from ML MoSe2 and the layered antiferromagnetic (AFM) semiconductor CrSBr, we show the formation of new exciton states depending on the twist angle. These excitons exhibit clear signatures of proximity coupling to the magnetic state of the AFM layer, such as hysteretic response to in- and out of plane B

fields. We discuss these results in the framework of Ising-type spin-orbit proximity coupling.

HL 31.8 Wed 12:15 H13

Shaped pulses enable robust coherent control of quantum dots: perspectives for quantum technologies — •Vikas Remesh — Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

Shaped laser pulses have been remarkably effective in investigating and controlling various light-matter interactions in a broad area of research. In quantum technologies, the techniques to shape complex spatiotemporal waveforms have found renewed interest, for instance in coherent control of quantum dots [1]. In this talk, I will navigate through the impact of pulse shaping techniques in nanospectroscopy and how it enabled efficient preparation schemes in quantum dots, based on our recent works [2], including the pioneering off-resonant coherent control of quantum dots, compact plug-and-play method of exciting multiple quantum dots and accessing dark excitons in quantum dots for advanced entanglement generation. Afterwards, I will conclude with my vision on the future scope of nanophotonics-assisted-quantum technology roadmap. [1] Photonic Quantum Technologies: Science and Applications 1, 53 (2023) [2] Nano Letters 22, 6567 (2022), Materials for Quantum Technology 3, 025006 (2023), APL Photonics 8, 101301 (2023), npj Quantum Information 10, 17 (2024), Advanced Quantum Technologies, 2300352 (2024), arXiv:2409.13981, arXiv:2406.07097, arXiv:2404.10708

HL 31.9 Wed 12:15 H13

First-Principles Investigation of NV Centers in Silicon Carbide Polytypes — •Timur Biktagirov, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Optically addressable spin defects in semiconductors offer versatile platforms for quantum applications, including computing, communication, and sensing. Among these, nitrogen-vacancy (NV) centers in silicon carbide (SiC) polytypes have emerged as a promising class of quantum defects, analogous to the NV center in diamond. In contrast to diamond, SiC is a technologically mature material with large-scale production capabilities, advanced doping techniques, and compatibility with CMOS fabrication methods. Additionally, the emission wavelengths of NV centers in SiC lie in the near-infrared range, making them particularly suitable for applications in single-photon emission. In this work, we discuss recent advancements in the ab initio investigation of NV centers in the 4H, 6H, and 3C polytypes of SiC. Simulating the magneto-optical properties of these spin centers, which are crucial for quantum applications, requires a detailed and accurate description of both the host material and the embedded defect. Accordingly, we demonstrate how supercell density functional theory (DFT) and recent implementations based on DFT can be employed to model key properties, including intra-defect optical transition energies, electron-electron and electron-nuclear spin interactions, and electron-phonon coupling. These theoretical insights provide a foundation for optimizing NV centers in SiC for next-generation quantum technologies.

HL 31.10 Wed 12:15 H13

Transport properties of quantum dots for single-electron pumps — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Frank Hohls, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, 31668 Braunschweig, Germany

A single-electron pump (SEP) is a device emitting a well-defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e, this results in a current of $I = nef$. Since the revision of the SI system, the elementary charge e hereby is an exact value, so that SEPs provide a suitable basis for a quantum current standard. The accuracy of this current is directly related to erroneous cycles, where the emitted number of electrons deviates from n. Our SEP devices are based on electrostatically defined quantum dots in GaAs/AlGaAs two-dimensional electron gases. In such devices, the tunnel barriers as well as the energy levels are controllable via gate voltages. Based on multiple quantum dot devices we here investigate relations between transport properties and SEP operation characteristics.

HL 32: Nitrides: Preparation and Characterization I

Time: Wednesday 9:30–11:00 Location: H15

HL 32.1 Wed 9:30 H15

Optical properties of asymmetric cubic AlGaN/GaN quantum wells — •Erik Graper[1], Elias Baron[1], Martin Feneberg[1], Tobias Wecker[2], Donat J. As[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany

Group III-nitrides, particularly AlGaN and GaN, are essential materials for high-performance electronic and optoelectronic devices. While conventional hexagonal AlGaN/GaN high-electron-mobility transistors (HEMTs) operate in normally-on mode, cubic AlGaN/GaN structures enable normally-off operation - a crucial advantage for energy-efficient power electronics. These cubic AlGaN/GaN heterostructures offer additional benefits such as the absence of internal polarization fields in (001) orientation.

In this study, we investigate asymmetric cubic AlGaN/GaN double quantum wells (2.5 nm and 0.6 nm) with varying barrier thicknesses, grown by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation. We employed complementary spectroscopic techniques to analyze quantum well coupling, combining photoluminescence (PL) measurements using continuous-wave lasers (266 nm and 325 nm) with photoluminescence excitation (PLE) spectroscopy using a tunable pulsed laser (325 - 354 nm). The acquired spectra were analyzed to determine wavelength dependent luminescence of the 2.5 nm quantum well.

HL 32.2 Wed 9:45 H15

Nanoscale characterization of cascaded GaN/InGaN LEDs with tunnel junction — •Konstantin Wein, Gordon Schmidt, Frank Bertram, Holger Eisele, Peter Veit, Olga August, Christoph Berger, Armin Dadgar, André Strittmatter, and Jürgen Christen — Otto-von-Guericke-University Magdeburg, Germany

In this work, comprehensive cathodoluminescence (CL) and electron beam induced current (EBIC) characterization directly performed in a scanning transmission electron microscopy (STEM) were performed on an InGaN/GaN double cascaded LED using a GaN:Ge/GaN:Mg tunnel junction (TJ). Cascaded LEDs benefit from monolithic multi-wavelength emission, lower injection current density (lower droop), and smaller chip sizes compared with standard LEDs. In low temperature (T = 17 K) highly spatially resolved CL, each individual layer is identified by its characteristic emission. The GaN:Si layers exhibit NBE emission at 365 nm corresponding to donor-bound exciton recombination, in contrast to the GaN:Mg layers which exhibit donor-acceptor pair recombination emitting at 380 nm. The intensity profile across the InGaN MQWs of both active regions gives access to the transport and capture of the excess carriers and excitons. The direct comparison of the local CL emission with the EBIC signal exhibits not only the local quantum efficiency as well as transfer of carriers (diffusion/drift) but also the current spreading/injection distribution of the vertical device. The impact of functional layers like electron blocking layers or TJs on the transport of carriers is directly visualized on the nano-scale.

HL 32.3 Wed 10:00 H15

Understanding the Effect of Defects in Ta3N5 Thin Films on Charge Carrier Dynamics — •Jan Luca Bläsdorf[1], Lukas M. Wolz[1], Matthias Kuhl[1], Johannes Dittloff[1,2], Nina Miller[1], Gabriel Grötzner[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany

Transition-metal nitrides are a highly interesting material space for solar-energy conversion due to their suitable bandgap for visible light absorption and high theoretical solar-to-hydrogen efficiencies. An intensively studied example is Ta3N5, with a bandgap of 2.2 eV and favorable band alignment for solar water splitting. However, its pho-

toelectrochemical performance is limited by oxygen impurities and nitrogen vacancies. Here, we used transient absorption spectroscopy on the microsecond timescale to reveal the impact of different defects on charge carrier dynamics in Ta3N5. Therefore, we synthesized Ta3N5 thin films with different concentrations of nitrogen vacancies and oxygen impurities. Their structure, defect and photoelectrochemical properties were correlated with charge carrier dynamics to identify current performance limitations.

HL 32.4 Wed 10:15 H15

Accessing and evaluating the full growth window of PAMBE grown AlGaN/GaN nanowires — •Rudolfo Hötzel[1], Marten Wilkens[1], Florian Krause[1], Andreas Rosenauer[1,2], Stephan Figge[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, 28359 Bremen, Germany

Typically group III/V nanowires synthesized by PAMBE are grown under a surplus of nitrogen. Under metal-rich conditions nanowire broadening is reported [1] leading to increased coalescence until self-stabilisation to stoichiometric conditions is reached. To establish stoichiometry single GaN nanowires consisting of multilayers of GaN grown with varying Ga fluxes were analyzed by STEM-EDX. The dependence of growth rates on temperature and fluxes could be consistently fitted with previously reported growth models [1] with the Ga desorption rate as the only free parameter. However a lateral broadening was not observed even for deep Ga-rich conditions. We attribute this to higher growth temperatures leading to an increased Ga desorption from the side facets. Based on these findings AlGaN/GaN nanowires were grown under deep metal-rich conditions. We observed that high Al/Ga fluxes lead to the formation of AlN regions due to the higher formation enthalpy of AlN with Ga accumulating on the c-face because of demixing. A homogenous incorporation of Al under deep metal-rich conditions was only possible for low Al/Ga flux ratios which are limited by the growth temperature. [1] S. Fernández-Garrido et al., Nano Lett. 13, 3274-3280 (2013)

HL 32.5 Wed 10:30 H15

Nanoscale multi-spectroscopic characterisation of InGaN pseudo-substrates grown on nanowire arrays — •Aidan Flynn Campbell, Jingxuan Kang, Huaide Zhang, Oliver Brandt, Lutz Geelhaar, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

The efficiency of nitride light-emitting diodes (LEDs) in the amber and red spectral ranges is severely limited by the high strain in (In,Ga)N quantum wells with increasing In content when grown on GaN. Thus, reducing the lattice mismatch between the active region and adjacent layers is highly desirable. Our approach exploits the lateral elastic strain relaxation facilitated by nanowires fabricated top-down from a single-crystalline layer, epitaxial overgrowth of a subsequent layer achieves a strain free pseudo-substrate. In this study, we characterise the optical, chemical, and crystallographic properties of such overgrown layers, which are key in understanding and optimising our epitaxial overgrowth fabrication route.

We utilise experimental techniques such as continuous-wave and time-resolved cathodoluminescence (TRCL), energy-dispersive X-ray spectroscopy (EDX), and high-resolution electron backscatter diffraction (HR-EBSD). We demonstrate low dislocation densities, low compositional variations and low crystal misorientation across coalescence boundaries. Furthermore, the factors influencing defect formation and the relevance of dislocation propagation are investigated and correlated with the resulting luminescence efficiency of the overgrown layers.

HL 32.6 Wed 10:45 H15

Measuring solute concentrations in ammonothermal solutions via in situ X-ray absorption - estimating detection limits for novel nitrides — •Rajesh Chirala, Ege N. Civas, and Saskia Schimmel — Chair of Electron Devices (LEB), Dept. EEI, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany

The ammonothermal method [1] is effective for producing high quality single crystals of binary and ternary nitrides [2], which are emerging semiconductor materials [3]. Despite the challenging process conditions (100 to 300 MPa, 400 to 800 °C), in situ measurement techniques such as X-ray imaging [4] allow to study reaction kinetics and solubilities, which are highly relevant to bulk crystal growth. In case of GaN, the quantitative determination of the concentration of Ga containing intermediates was already demonstrated [5].

By simulating the X-ray absorption of novel nitrides in an ammonothermal autoclave, we estimate element-specific detection limits for solute concentrations and derive strategies for detecting lighter elements or lower concentrations. Amongst the others, effectiveness of using a combination of lower X-ray energies and higher X-ray dose will be analyzed.

References :-
[1] R. Dwilinski et al., Acta Phys. Pol. A 88, 833, 1995.
[2] J. Häusler, W. Schnick, Chemistry 24, 11864, 2018.
[3] D. Jena et al., Jpn. J. Appl. Phys. 58, SC0801, 2019.
[4] S. Schimmel et al., J. Cryst. Growth 418, 64, 2015.
[5] S. Schimmel et al., J. Cryst. Growth 498, 214, 2018.

HL 33: Nitrides: Devices

Time: Wednesday 11:15–13:00 Location: H15

HL 33.1 Wed 11:15 H15

Influence of barrier height variations on the efficiency of AlGaN-based 225nm LEDs — •Markus A. Blonski[1], Jakob Höpfner[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[2], Paula Vierck[1], Tim Wernicke[1], Michael Kneissl[1,2], and Markus Weyers[2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Deep ultraviolet (DUV) light emitting diodes (LEDs) with emission wavelengths shorter than 225 nm exhibit low external quantum efficiencies (EQEs). Since the AlGaN multi-quantum well (MQW) active region remains a significant limiting factor for EQE, the effects of the barrier height in the MQW region on the radiative recombination efficiency (RRE), carrier injection efficiency (CIE) and light extraction efficiency (LEE) are examined. For this, the barrier composition is varied from $Al_{0.82}Ga_{0.18}N$ over $Al_{0.86}Ga_{0.14}N$ to $Al_{0.89}Ga_{0.11}N$. The lowest barrier leads to the highest peak EQE at 0.05 % and the highest barrier to an EQE peak below 0.02 %. The RRE, CIE and LEE are determined using continuous wave and pulsed electroluminescence measurements, determination of optical polarization and Monte Carlo raytracing simulations. The analysis shows that an increase in barrier height leads to an increase in RRE and LEE and a significant decrease in CIE for an overall decrease in EQE. Drift diffusion simulations indicate a notable increase in electron spillover across the $Al_{0.98}Ga_{0.02}N$ electron blocking layer to the p-side, attributable to a reduced band offset between barrier and electron blocking layer, reducing the CIE.

HL 33.2 Wed 11:30 H15

Homoepitaxy on AlN-bulk substrates with different off-cut angles — •Sebastian Krüger[1], Sarina Graupeter[1], Massimo Grigoletto[1,2], Marcel Schilling[1], Sylvia Hagedorn[2], Carsten Hartmann[3], Thomas Straubinger[3], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Laser diodes in the UVC spectral range require high-quality AlN and AlGaN layers with low threading dislocation densities (TDD) and smooth surfaces. AlN substrates with a TDD of $< 10^4$ cm^{-2} are the ideal choice. In this work we investigate the influence of substrate off-cut (0.1° to 0.5°) and growth parameters (e.g. TMAl flow, V/III-ratio) on the morphology of homoepitaxially grown AlN buffer layers. A transition from step flow growth for a 0.2° miscut AlN substrate to step bunching for miscuts of 0.39° and above is observed for a growth temperature of 1070°C, a TMAl flow of 35 μmol/min and a V/III-ratio of 15. For a miscut of 0.27° step flow growth is still present but the terrace width shows significant variation. The RMS roughness increases from 0.11 nm (on 0.2°) to 0.45 nm (on 0.39°). For 0.5° miscut, the substrate terrace width is even smaller, i.e. the diffusion length must be reduced to avoid step bunching e.g. by increasing the V/III-ratio. Between V/III ratios of 15 and 60 we found morphologies such as is-

land growth and step meandering with the lowest RMS roughness of 0.11 nm for a TMAl flow of 35 μmol/min and a V/III-ratio of 15.

HL 33.3 Wed 11:45 H15

Stabilizing Ta_3N_5 Thin Films Photoelectrodes by Defect Engineering — •Lukas M. Wolz[1], Gabriel Grötzner[1,2], Tim Rieth[1,2], Laura I. Wagner[1,2], Matthias Kuhl[1], Johannes Dittloff[1,2], Guanda Zhou[1,2], Saswati Santra[1,2], Verena Streibel[1,2], Frans Munnik[3], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Tantalum nitride (Ta_3N_5) is a highly investigated photoelectrode material due to its favorable optoelectronic properties for photoelectrochemical (PEC) energy conversion. However, intrinsic defects such as nitrogen vacancies and oxygen impurities play a crucial role in defining their optical, electronic, and photoelectrochemical properties. While the role of these defects in PEC activity is well investigated, their impact on material stability remains underexplored. We investigate the relationship between atomic-scale defects and macroscale PEC stability in Ta_3N_5 thin films. To reveal the impact of each defect type on the material properties, we introduced different defect concentrations in Ta_3N_5 by using three different precursors in the synthesis process. Low oxygen concentrations are found to increase long-range order but lead to high concentrations of deep-level defects, leading to increased charge recombination and decreased material stability. Conversely, higher oxygen contents result in reduced structural order but beneficially passivate deep-level defects, leading to improved stability.

HL 33.4 Wed 12:00 H15

Studying the carrier distribution of multicolor far-UVC LEDs by temperature dependent electroluminescence measurements — •Jakob Höpfner[1], Franz Biebler[1], Florian Kühl[1], Marcel Schilling[1], Anton Muhin[1], Massimo Grigoletto[1,2], Martin Guttmann[2], Gregor Hoffmann[3], Friedhard Römer[3], Tim Wernicke[1], Berndt Witzigmann[3], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), 12489 Berlin, Germany — [3]Lehrstuhl für Optoelektronik, Department EEI, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

The low current injection efficiency (CIE) is one of the root causes for the poor external quantum efficiency of AlGaN based far-UVC LEDs. To improve the CIE it is necessary to gain insights into the carrier distribution and transport in the AlGaN multiple quantum well active region. Therefore, heterostructures were grown by metalorganic vapour phase epitaxy (MOVPE) with a varying number of QWs (2 –20) emitting at 233 nm and one single QW with an emission wavelength of 250 nm. This allows us to probe the carrier transport with the help of temperature dependent electroluminescence measurements (100 K - 340 K). The experimental findings were correlated with drift-diffusion simulations and Monte-Carlo ray-tracing simulations. Experiment and simulations show that the holes are weakly confined in the 233 nm emitting QWs and exhibit a long diffusion length over many QWs mainly due to thermal escape from the shallow barriers.

HL 33.5 Wed 12:15 H15

Influence of strain reduced HTA-AlN/sapphire templates with different offcuts on the performance of UVC LEDs — •Sarina Graupeter[1], Finn Kusch[1], Paula Vierck[1], Sylvia Hagedorn[2], Markus Weyers[2], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

High temperature annealing (HTA) of sputter dposited AlN layers on (0001) sapphire substrates allows for fabrication low threading dislocation densitiy templates (TDD of 4 x $10^8 cm^2$) enabling UVC LEDs with improved external quantum efficiency and lifetime. However, due to the thermal expansion mismatch of the sapphire and the AlN, the AlN layers are under high compressive strain after cooling down from HTA at 1700°C. This can lead to strain relaxation and formation of dislocation half-loops during the subsequent growth of AlN and AlGaN layers, thus decreasing the radiative recombination efficiency (RRE). By growing a Si-doped AlN layer on HTA-AlN the in-plane compressive strain ϵ_{xx} is reduced by around 30% from -0.3 to -0.2. The impact of such an interlayer on the electro-optical properties of UVC-LEDs has been investigated with focus on the RRE. The RRE has been determined using cw and pulsed EL-measurements with the Titkov-Dai method. Using an AlN:Si interlayer shows an increase of the EQE value from 0.8% to 1%. Emission powers as high as 1.9 mW at 50 mA can be realized for UVC LEDs on strain reduced templates.

HL 33.6 Wed 12:30 H15

Characterisation of a Pt on-chip counter electrode on a GaN/AlGaN-ISFET Wheatstone bridge as pH-sensor — •Alexander Hinz[1], Niklas Krantz[1], Stephan Figge[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany

The influence of a Pt on-chip counter electrode on field effect transistors as pH-sensors was investigated. The intention was to reduce the size of the complete sensor structure consisting of ISFET, counter and reference electrode. In addition, the function of the Pt on-chip electrode was be compared to setup using an external Pt counter electrode to discuss stability and leakage. Furthermore, a Wheatstone bridge design is used to compensate temperature drifts. A reduction of this drift to 0.02 mV/°C was achieved. The long-time behavior of the temperature drift and also of pH changes was also analysed.

HL 33.7 Wed 12:45 H15

Efficiency analysis of 233 nm far-UVC LEDs with varied DPD AlGaN layer thickness beyond 298 K — •Paula Vierck[1], Jakob Höpfner[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Markus Blonski[1], Tim Wernicke[1,2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand Braun Institut (FBH), Berlin, Germany

Light emitting diodes (LEDs) emitting in the far ultraviolet-C (far-UVC) spectral range offer applications in skin safe disinfection and gas sensing. In this work we analyze far-UVC LEDs with a distributed-polarization doped (DPD) p-AlGaN layer as this offers a promising alternative to Mg-doping. By compositionally grading the Al content of the AlGaN layer, a 3D hole gas can be generated exceeding the free hole concentration of conventionally Mg doped samples. The theoretically calculated charge profile depends on the grading and can be controlled by changing the DPD layer thickness or the alloy composition. In this work, five samples with DPD layer thicknesses between 25 nm and 150 nm were investigated by electroluminescence spectroscopy and numerical simulations. With decreasing DPD layer thickness we find an increase in the peak external quantum efficiency (EQE) with a maximum EQE of 0.37 % for a DPD thickness of 25 nm due to an increased hole concentration. Further analysis at temperatures of up to 353 K revealed a notable decline in the devices EQE down to 0.15 % at 353 K for a 25 nm thick DPD. This work will provide an analysis of the different contributing factors to the EQE drop with insights provided by simulations.

HL 34: Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)

In this joint focused session of the divisions DY, HL, and TT, we bring together two dynamic areas of research: semiconductor quantum emitters and chaotic cavities. While quantum emitters in cavities represent an established building block for quantum information technologies, chaotic microcavities may promise novel design routes towards optimized cavity performance parameters. Experts from both fields will provide an overview of the current state of research, exploring the potential of chaotic and unconventional microcavities to enhance the emission of quantum states.

Organized by Sonja Barkhofen (University of Paderborn) and Christian Schneider (University of Oldenburg).

Time: Wednesday 9:30–12:15 Location: H17

Invited Talk HL 34.1 Wed 9:30 H17

From complex internal dynamics to emission characteristics control in quantum billiards — •Martina Hentschel — 1 Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

The field of mesoscopic physics has given access to new classes of fascinating model systems ranging from ballistic quantum dots via microcavity lasers to graphene billiards over the past decades. Their rich internal dynamics, subject to quantum chaos and often successfully accessed employing wave-particle correspondence in real and phase space, is directly related to their emission properties. Here, we illustrate this close connection for various examples and system classes. For optical microcavities, we vary the internal dynamics by changing the geometric shape of the resonator and explain how the far-field emission characteristics is determined by the underlying steady probability distribution and a possibility to achieve directional emission required for microlasing devices with the Limaçon geometry. Placing sources into the cavity will affect the internal dynamics of the cavity by, taking the particle point-of-view, effectively changing the set of initial conditions, as observed for optical cavities as well as for graphene billiards in the form of Dirac fermion optics. A further way to change the dynamics of a system is the existence of anisotropies that can either be intrinsically present such as in bilayer graphene in the form of trigonal warping [1], or can be induced to a given system by, for example, applying a mechanical strain. [1] L. Seemann, A. Knothe, and M. Hentschel, New J. Phys. 26, 103045 (2024).

Invited Talk HL 34.2 Wed 10:00 H17

Positioning of microcavities around single emitters — •Tobias Huber-Loyola — Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Single emitters in solids are great sources of single and entangled photons for usage in quantum information technologies. Many emitters possess high internal quantum efficiency, majority of the emission into the zero-phonon line and controllable single charge spins that can be used as quantum memories or as resource to generate chains of entangled photons. However, due to their solid-state host, which usually comes with a high refractive index, the outcoupling of photons requires the use of nanophotonic structures such as waveguides or microcavities. In this talk, I will show how we place microcavities around pre-registered quantum dots using hyperspectral imaging and e-beam lithography and I will give an overview of how placement accuracy has different effects on the emitted photons‘ properties based on the type of cavity.

Invited Talk HL 34.3 Wed 10:30 H17

Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities — •Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, Germany

Optical microcavities play a fundamental role in many fields of basic and applied research in physics. A chaotic microcavity is a type of cavity where the light ray dynamics is (partially) chaotic [1]. This can occur in a microdisk cavity with a deformed boundary shape. Chaotic microcavities are ideal for studying ray-wave correspondence, or wave chaos, in open systems, allowing direct comparisons with experiments [2]. These cavities can also exhibit non-Hermitian phenomena such as reflectionless scattering modes [3] and exceptional points [4].

The light emission from chaotic microcavities has been studied exclusively within the classical domain. The effects of electromagnetic field quantization, including phenomena like entanglement, single-photon states, and squeezed light, remain unexplored in this context. In this talk, I will review my group's recent efforts to investigate classical emission from chaotic microcavities and quantum emission from semiconductor quantum dots embedded in conventional microcavities. Additionally, I will discuss the prospects for achieving genuine quantum emission from chaotic microcavities.

[1] H. Cao and J. Wiersig, Rev. Mod. Phys. 87, 61 (2015)
[2] X. Jiang et al., Science 358, 344 (2017)
[3] X. Jiang et al., Nat. Phys. 20, 109 (2023)
[4] C.-H. Yi et al., Phys. Rev. Lett. 120, 093902 (2018)

15 min. break

Invited Talk HL 34.4 Wed 11:15 H17

Correlations and statistics in cavity embedded quantum dot sources of quantum light — •Ana Predojevic — Stockholm University, Stockholm, Sweden

Single quantum dots coupled to photonic cavities are established emitters of single photons and entangled photon pairs. The cascaded generation of photon pairs intrinsically contains temporal correlations that negatively affect the ability of such sources to perform two-photon interference, hindering applications. I will show how such correlation interacts with decoherence and temporal postselection, and under what conditions temporal postselection could improve two-photon interference visibility. Our study identifies crucial parameters of the source and shows the way to achieve optimal performance. The single photons emitted by a quantum dot exhibit quantum statistics, which is usually verified in an autocorrelation measurement. Single photons can be subjected to more extensive tests of quantum nature, such as non-Gaussianity. However, there is little evidence that such a measurement can be made on pairs of photons. I will show that pairs of photons exhibit strongly non-classical properties that can be quantified. Our result is applicable to a wide range of quantum light sources and measurement methods.

Invited Talk HL 34.5 Wed 11:45 H17

Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum — •Dario Ballarini — CNR-NANOTEC, Lecce, Italy

Exciton-polaritons in semiconductor microcavities have demonstrated remarkable collective behaviors and nonlinear interactions. In this work, we introduce an alternative platform to study strong light-matter interactions within a waveguide configuration. Among other interesting phenomena and applications, such as dispersion engineering of waveguide exciton-polaritons or exciton tuning through the Stark effect [1,2], we highlight the demonstration of parametric nonlinearities, polariton lasing from bound-in-the-continuum (BIC) states, and the recent realization of polariton BICs operating at room temperature in 2D materials [3-5].

[1] Electrically controlled waveguide polariton laser, Optica 7, 1579 (2020). [2] Reconfigurable quantum fluid molecules of bound states in the continuum, Nature Physics 20, 61 (2024). [3] Polariton Bose-Einstein condensate from a bound state in the continuum, Nature 605, 447 (2022). [4] Emerging supersolidity from a polariton condensate in a photonic crystal waveguide, arXiv:2407.02373 (2024). [5] Strongly enhanced light-matter coupling of monolayer WS2 from a bound state in the continuum, Nature Materials 22, 964 (2023).

HL 35: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

HL 35.1 Wed 10:30 H11

The Bell-Shaped Component in Diffraction from 2D Materials — •Birk Finke[1], Christian Brand[1], Karim Omambac[1,2], Pascal Dreher[1], Hannah Kohler[1], Frank-J. Meyer zu Heringdorf[1,3,4], and Michael Horn-von Hoegen[1,3] — [1]Universität Duisburg-Essen — [2]Polytechnique Montréal Canada — [3]Center for Nanointegration Duisburg-Essen — [4]Interdisciplinary Center for Analytics on the Nanoscale

In 2D materials, the formation of moiré superlattices with graphene or hBN on crystalline surfaces alters electronic, vibrational, and chemical properties. Here we analysed an unusual broad diffraction background observed in low energy electron diffraction from 2D material systems, which is called the bell-shaped component (BSC). Employing SPA-LEED, LEEM, and μ-LEED we propose the origin to be the inelastic scattering of the low energy electrons at the vertically polarized ZA-phonons of the weakly bound graphene and hBN layers on Ir(111) and SiC(0001). For these systems the ZA-phonon branch exhibits a parabolic dispersion with a finite phonon frequency of a few meV at the Γ point. This results in a high phonon density at low energy, but high momentum causing the strong intensity of the BSC in diffraction. In the framework of kinematic scattering theory, we performed simulations of the inelastic diffuse scattering which quantitively confirm our proposal.

HL 35.2 Wed 10:45 H11

Combining DFT and ML to Explore the Electronic Properties of Nano-porous Graphene — •Bernhard Kretz and Ivor Lončarić — Institut Ruder Bošković, Zagreb, Croatia

Nano-porous graphene (NPG) holds great potential in electronics due to its tunable electronic properties. However, establishing a comprehensive understanding of how structural parameters influence these properties remains a challenge. This work employs density functional theory (DFT) calculations combined with machine learning (ML) to systematically investigate both static and dynamic electronic properties across a set of 460 NPG structures derived from four distinct templates.

Our DFT results reveal correlations between structural features and band gaps within subsets of our NPG structures. Notably, we identify certain NPG configurations exhibiting band gap behavior analogous to armchair graphene nano-ribbons. To predict the dynamic response of our NPG structures, we train two distinct ML networks: one for predicting forces and total energies, and another one for predicting band gaps. Using the former allows us to perform temperature-dependent molecular dynamics simulations for all 460 NPG structures, while the latter enables us to predict band gap evolution under varying operating temperatures, a crucial factor for semiconductor device performance. Our findings identify several NPG structures exhibiting band gaps suitable for semiconductor applications while demonstrating sufficient thermal stability to function effectively at typical operating temperatures.

Invited Talk HL 35.3 Wed 11:00 H11

Polaritons in two-dimensional materials and hybrids probed by electron beams — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel

Polaritonic quasiparticles in two-dimensional (2D) materials have garnered significant attention in recent years, emerging as a promising platform for studying novel photon- and phonon-mediated correlations between various material excitations. In this work, we employ electron beams to investigate exciton and plasmon polaritons in diverse 2D materials, including transition-metal dichalcogenides, perovskites, hexagonal boron nitride, borophene, and hybrid systems. By comparing cathodoluminescence and photoluminescence spectroscopy, we uncover differences in the selection rules governing the excitation of quasiparticles by coherent light versus electron beams. Furthermore, leveraging a recently developed method that utilizes electron-driven photon sources inside an electron microscope for Ramsey-type spectroscopy, we examine the coherence of cathodoluminescence emitted by exciton polaritons (Nature Physics 19, 869 (2023)) and defects in hexagonal boron nitride (arXiv:2404.09879). These results provide new insights into the temporal coherence of the radiation from 2D materials excited by coherent and incoherent excitations.

HL 35.4 Wed 11:30 H11

Electron-phonon interaction in polar two-dimensional materials — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We recently developed a generally applicable ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation, which are usually neglected [1].

Incorporating effects from macroscopic electric fields into our implementation allows us to extend our calculations to the class of polar materials. In this presentation we discuss our results for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

HL 35.5 Wed 11:45 H11

Structural modulations of unidirectional charge density waves in rare earth tellurides — •Eunseo Kim[1], Sanghun Lee[1], Junho Bang[1], Hyungryul Yang[1], Jongho Park[2], Changyoung Kim[2], Dirk Wulferding[2], Doohee Cho[1], Makoto Hashimito[3], Donghui Lu[3], and Sunghun Kim[4] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea — [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Department of Physics, Ajou University, Suwon 16499, Korea

Charge density waves (CDWs) in rare earth tellurides (RTe_3) provide a unique platform for exploring the interplay between lattice deformations and electronic order. Using scanning tunneling microscopy and spectroscopy (STM/S), we investigate unique surface features in two different materials, $GdTe_3$ and $DyTe_3$, that influence the CDW behavior. In $GdTe_3$, twin domain boundaries provide a static platform for observing the spatial "melting" of unidirectional CDWs and the emergence of bidirectional CDWs. Our spatial lock-in analysis demonstrates the attenuation of CDW order parameters and the proliferation of topological defects at these boundaries, correlating with enhanced local density of states near the Fermi level. In $DyTe_3$, nanowrinkles act as topological interfaces, hosting phase-winding CDWs and confining one-dimensional metallic states. These findings emphasize the role of local structural distortions in shaping CDW phenomena, offering insights into manipulating quantum states via lattice engineering.

HL 35.6 Wed 12:00 H11

Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field — •Jan-Philip Joost and Michael Bonitz — Kiel University, Institute for Theoretical Physics and Astrophysics, 24098 Kiel, Germany

When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [1]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [2]. Further, we demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects greatly benefit from surface screening, while in free-standing systems the targeted charge

excitation is restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

[1] J.-P. Joost et al., Nano Lett. **19**, 9045 (2019)
[2] J.-P. Joost et al., Phys. Rev. B **105**, 165155 (2022)

HL 35.7 Wed 12:15 H11

Two-dimensional breathing Kagome lattice of antimony atoms on a SiC substrate — •Bing Liu[1], Kyungchan Lee[1], Jonas Erhardt[1], Manish Verma[1], Stefan Enyner[1], Cedric Schmitt[1], Philipp Kessler[1], Lukas Gehrig[1], Chris Jozwiak[2], Aaron Bostwick[2], Martin Kamp[1], Eli Rotenberg[2], Jörg Schäfer[1], Simon Moser[1], Giorgio Sangiovanni[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The Kagome lattice, characterized by flat electronic bands, which represents a class of candidate materials for charge order, time-reversal symmetry-breaking and exotic superconductivity. In this work, we report the successful synthesis of a breathing Kagome lattice of Sb on SiC surface. Band mapping reveals a significant gap opening at the K point near the Fermi level, driven by different hopping parameters within the breathing Kagome lattice. Scanning tunneling microscopy measurements of this phase confirm a well-ordered 2x2 lattice reconstruction, consistent with the breathing Kagome unit cell. Furthermore, DFT calculations elucidate the role of the Sb p-orbitals. Specifically, near the Fermi level the physics is dominated by px and py orbitals, which are sensitive to hopping and possibly electron correlation, giving rise to an energy gap, and by their splitting reflect the breathing Kagome lattice situation. Our findings demonstrate a pathway for constructing two-dimensional Kagome lattices on semiconductor surfaces, and are encouraging further research into their spin and electronic properties.

HL 35.8 Wed 12:30 H11

Ultrafast lattice dynamics of monolayer ReS_2 — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Within the transition metal dichalcogenide (TMDC) material family, TMDCs containing rhenium stand out due to their low crystal symmetry. Instead of the common hexagonal structure, ReS_2 exhibits in-plane 1D chains of rhenium ions due to a Peierls-like distortion. This highly anisotropic crystal structure results in a range of material properties, such as anisotropic effective carrier masses, polarization dependent optical absorption, and extremely weak interlayer coupling.

We present femtosecond electron diffraction (FED) measurements of monolayer ReS_2. FED is a direct probe of photoexcited lattice dynamics, providing quantitative information on coherent and incoherent atomic vibrations on femtosecond timescales. In ReS_2 monolayers we observe a strong and complex lattice response to photoexcitation. In particular, we observe a rapid ($<$1 ps) collective response, indicative of a concerted change in ionic positions within the unit cell. We measure the fluence dependence of this response and investigate the effect of the pronounced polarization dependence of the optical excitation, which results from the material's in-plane anisotropy.

HL 36: Materials and Devices for Quantum Technology II

Time: Wednesday 15:00–18:00 Location: H13

HL 36.1 Wed 15:00 H13

High aspect ratio wurtzite GaAs nanowires as a platform for hexagonal SiGe — •Marvin Marco Jansen[1], Wouter H.J. Peeters[1], Marcel A. Verheijen[1,2], and Erik P.A.M. Bakkers[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherland — [2]Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands

One of the most promising pathway to create a silicon based laser is the recently developed hexagonal silicon germanium (hex-SiGe) shells around wurtzite (WZ) gallium arsenide (GaAs) nanowires (NWs) for which efficient direct band gap emission was shown. However, studies have highlighted the limitations of the core/shell NW system. A main challenge is the recently discovered aspect ratio limitation in WZ GaAs NWs ascribed to a dynamic variation of the growth conditions. Here, we report on the crystal phase control of GaAs NWs down to the monolayer regime opening up new pathways for superlattices as well as high aspect ratios GaAs NWs. To achieve this, Ga pulses are executed by momentarily halting the As supply, leading to an accumulation of Ga atoms within the catalyst particle. This process leads to the increase of the contact angle of the catalyst particle enabling a controlled transition from the WZ phase to the zinc blende (ZB), and then back to the WZ phase. By using the ZB inclusion as a marker during the growth process, we successfully carried out a detailed investigation into the evolution of the NW growth, considering its diameter, length, and the pulse frequency.

HL 36.2 Wed 15:15 H13

Shaped pulses enable robust coherent control of quantum dots: perspectives for quantum technologies — •Vikas Remesh — Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

Shaped laser pulses have been remarkably effective in investigating and controlling various light-matter interactions in a broad area of research. In quantum technologies, the techniques to shape complex spatiotemporal waveforms have found renewed interest, for instance in coherent control of quantum dots [1]. In this talk, I will navigate through the impact of pulse shaping techniques in nanospectroscopy and how it enabled efficient preparation schemes in quantum dots, based on our recent works [2], including the pioneering off-resonant coherent control of quantum dots, compact plug-and-play method of exciting multiple quantum dots and accessing dark excitons in quantum dots for advanced entanglement generation. Afterwards, I will conclude with my vision on the future scope of nanophotonics-assisted-quantum technology roadmap. [1] Photonic Quantum Technologies: Science and Applications 1, 53 (2023) [2] Nano Letters 22, 6567 (2022), Materials for Quantum Technology 3, 025006 (2023), APL Photonics 8, 101301 (2023), npj Quantum Information 10, 17 (2024), Advanced Quantum Technologies, 2300352 (2024), arXiv:2409.13981, arXiv:2406.07097, arXiv:2404.10708

HL 36.3 Wed 15:30 H13

Single-Electron Shuttling for Scalable Silicon Quantum Computers: Modeling, Simulation and Optimal Control — •Lasse Ermoneit[1], Burkhard Schmidt[1], Thomas Koprucki[1], Jürgen Fuhrmann[1], Tobias Breiten[2], Arnau Sala[3], Nils Ciroth[3], Ran Xue[3], Lars R. Schreiber[3,4], and Markus Kantner[1] — [1]Weierstrass Institute, Berlin, Germany — [2]Technical University Berlin, Germany — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Germany — [4]ARQUE Systems GmbH, Aachen, Germany

While spin qubits in gate-defined Si/SiGe quantum dots provide excellent prospects for scalability, the lithographic processing, signal routing and wiring of large qubit arrays at a small footprint pose a significant challenge. A potential solution is to divide the qubit register into compact, dense qubit arrays linked by an interconnecting quantum bus shuttle, that allows for coherent transfer of quantum information by physically moving electrons along a channel. Limitations in qubit shuttling fidelity arise from the interaction of the electron with material defects within the channel that can cause non-adiabatic transitions to excited orbital states. Since those have an altered effective g-factor, this leads to a spin precession with an indeterministic phase. In this contribution, we theoretically explore the capabilities for bypassing defect centers using optimally engineered control signals that allow for a quasi-adiabatic passage of the electron through the channel without reducing the shuttling velocity. Our approach is based on quantum optimal control theory and Schrödinger wave packet propagation.

HL 36.4 Wed 15:45 H13

Spectral Hole linewidths and donor-acceptor dynamics in ultra-pure 28-Si:P — •Nico Eggeling[1], Finja Tadge[1], N.V.

Abrosimov[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

Donor-bound excitons in ultra-pure silicon show significant inhomogeneous broadening, which can be studied in detail using spectral hole burning[1]. Surprisingly, for decreasing pump intensities, the linewidth of these holes does not approach the natural transition linewidth, resulting from the dominating Auger effect at low temperatures[2]. Instead, time-dependent experiments show that the width and decay of the spectral holes change significantly with temperature and magnetic field, which an intricate model including donor-acceptor pair recombination can explain.

[1] J. J. Berry, et al. Appl. Phy. Lett. **88**, 061114, (2006).
[2] Yang, et al. Appl. Phy. Lett. **95**, 122113, (2009).

HL 36.5 Wed 16:00 H13

The Kitaev transmon qubit: design, readout and operation — •Tobias Kuhn and Monica Benito — Augsburg University, Augsburg, Germany

Fermionic-parity qubits are very stable but cannot be operated in isolation. Coupling two parity qubits allows us to construct parity-spin qubit states within one global parity [1]. Its degeneracy and nonlocality should improve T_2 and T_1 times [2]. A parity qubit can be realized in a double quantum dot connected via a common superconducting lead, where elastic cotunneling t as well as crossed Andreev reflection Δ preserve parity. This minimal Kitaev chain possesses degenerate distinct-parity states at the sweetspot $\Delta = t$[1]. Weakly coupling two minimal Kitaev chains inside a transmon loop introduces an additional Josephson potential which is a consequence of the emerging parity-spin qubit [3]. This hybrid device combines the advantages of both quantum dots and transmons to promise a high-fidelity qubit device we call Kitmon (Kitaev transmon). We theoretically analyze even and odd global parity subspaces of the Kitaev junction and show that flux spectroscopy in a circuit QED implementation [4] determines global parity. Additionally, we derive an effective Hamiltonian depending on the transmon excitation state, which is useful for single qubit operations and qubit readout. [1] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012) [2] G.-L. Guo, H.-B. Leng, and X. Liu, New J. Phys. **26**, 063005 (2024) [3] D. M. Pino, R. S. Souto, and R. Aguado, Phys. Rev. B **109**, 075101 (2024) [4] L. Peri, M. Benito, C. J. B. Ford, and M. F. Gonzalez-Zalba, npj Quantum Inf **10**, 1 (2024)

HL 36.6 Wed 16:15 H13

Towards the goal of reliably storing single-photons from a quantum dot — •Ioannis Caltzidis[1], Patricia A. Kallert[1], Chase Wallace[2], Sean Keenan[3], Nicolas Claro-Rodríguez[1], Santiago Bermúdez-Feijóo[1], Sonja Barkhofen[1], Margherita Mazzera[3], Eden Figueroa[2], and Klaus D. Jöns[1] — [1]Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP) and Department of Physics, Paderborn University, Germany — [2]Quantum Memories Group, Heriot-Watt University, Edinburgh, Scotland, United Kingdom — [3]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA and Brookhaven National Laboratory, Upton, NY, USA

In quantum networks, precise single-photon arrival times are crucial for effective entanglement swapping protocols. Therefore, quantum memories are curcial to store photons until read out simultaneously and synchronously routed to further processing, e.g. Bell measurements. To operate a varm vapor memory in our laboratories we present initial results demonstrating our ability to generate short optical pulses in the desired frequency domain optimized for the atomic transitions of rubidium. We further probe the interaction of short pulses with the atomic medium in the presence or absence of different supsidiary lightfields. This series of experiments aims to probe the parameter space of our system with the goal of storing single photons fom quantum dots in a rubidium based EIT Memory.

15 min. break

HL 36.7 Wed 16:45 H13

Stability of Majorana modes in disordered topological insulator nanowires — •Leonard Kaufhold — Institute for theoretical physics, Cologne, Germany

The possibility of Majorana bound states (MBS) in nanowire hybrid devices has sparked great interest over the past decade due to their potential application in quantum computing. In this talk, we evaluate theoretically the possibility to realize MBS in topological-insulator (TI) nanowires proximity-coupled to an s-wave superconductor with regards to one main obstacle: disorder, be it from charged impurities within the bulk of the TI or short ranged surface defects. Based on extensive numerical investigation of screening effects as well as the resulting surface states, we demonstrate, that Majorana modes can be achieved under realistic conditions.

HL 36.8 Wed 17:00 H13

Signature of topological transitions in Na-Sb-Bi alloys via Compton scattering — •Aki Pulkkinen[1], Veenavee Kothalawala[2], Kosuke Suzuki[3], Bernardo Barbiellini[2,4,5], Hiroshi Sakurai[3], Ján Minár[1], and Arun Bansil[4,5] — [1]New Technologies-Research Centre, Pilsen, Czech Republic — [2]School of Engineering Science, LUT University, Finland — [3]Graduate School of Science and Technology, Gunma University, Japan — [4]Department of Physics, Northeastern University, USA — [5]Quantum Materials and Sensing Institute, Northeastern University, USA

We investigate the topological transition in Na-Sb-Bi alloys using x-ray Compton scattering experiments, combined with first-principles modeling of the electronic structure. A robust signature of the semiconductor-to-Dirac semimetal transition is identified in the spherically averaged Compton profile. We demonstrate the evolution of the electronic structure across the topological transition as a function of Bi concentration using the coherent potential approximation (CPA) within the fully relativistic, full potential Korringa-Kohn-Rostoker (KKR) method implemented in the SPRKKR package. Spherically averaged Compton profiles are estimated by averaging over directional profiles over a set of special directions within the KKR method. We demonstrate how the number of electrons involved in the topological transition can be estimated, providing a new descriptor to quantify the strength of the spin-orbit coupling driving the transition. Our study also highlights the sensitivity of the Compton scattering technique in capturing the spillover of Bi 6p relativistic states onto Na sites.

HL 36.9 Wed 17:15 H13

Circular photonic crystal grating design for charge-tunable quantum light sources in the telecom C-band — •Chenxi Ma[1], Jingzhong Yang[1], Pengji Li[1], Eddy Rugeramigabo[1], Michael Zopf[1], and Fei Ding[1,2] — [1]Leibniz University Hannover, Institute of Solid State Physics, Hannover, Germany — [2]Leibniz University Hannover, Laboratory of Nano and Quantum Engineering, Hannover, Germany

Efficient generation of entangled photon pairs at telecom wavelengths is a key ingredient for long-range quantum networks. While embedding semiconductor quantum dots into hybrid circular Bragg gratings has proven effective, it conflicts with p-i-n diode heterostructures which offer superior coherence. We propose and analyze hybrid circular photonic crystal gratings, incorporating air holes to facilitate charge carrier transport without compromising optical properties. Through numerical simulations, a broad cavity mode with a Purcell factor of 23 enhancing both exciton and biexciton transitions, and exceptional collection efficiency of 92.4

HL 36.10 Wed 17:30 H13

Control of NV centre generation in pulsed plasma chemical vapor deposition (CVD) grown diamonds — •Ravi Teja Aditya[1], Felix Hoffmann[1], Patrik Stranak[1], Volker Cimalla[1], and Rüdiger Quay[1,2] — [1]Fraunhofer Institute for Applied Solid State Physics, Tullastraße 72, D-79108 Freiburg, Germany — [2]Department for Sustainable Systems Engineering INATECH, University of Freiburg, 79108 Freiburg, Germany

Nitrogen vacancy (NV) centres in diamond have emerged to be an integral part in many quantum computing and quantum sensing applications. High and precise NV density is required especially for quantum sensing applications. There is a need for control of nitrogen incorporation and NV yield without compromising crystal quality and growth rate. Although higher power levels ensure higher nitrogen incorporation, it is often limited by temperature. Investigating pulsed plasma chemical vapor deposition (CVD) for this purpose proved to be beneficial to control the NV generation. A pulsed plasma generator was used to reach higher power levels while maintaining an appropriate temperature by adjusting the duty cycle accordingly. Time resolved optical emission spectroscopy (OES) was used to observe the plasma composition during microwave pulses. A pulse length dependent activation of CN radicals was observed which led to a variation in NV densities in grown films. We present the results of variation of NV densities in diamond films caused by variation in pulse length, MW

power and duty cycle.

HL 36.11 Wed 17:45 H13

Charge-tunable quantum dot single photon sources for quantum repeater experiments — •Peter Gschwandtner, Quirin Buchinger, Constantin Krause, Sebastian Krüger, Silke Kuhn, Tobias Huber-Loyola, and Sven Höfling — Julius-Maximilian-Universität Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik, Germany

Semiconductor quantum dots (QD) are promising candidates for entangled photon sources (SPS) for quantum network purposes [1]. Single charge spins in QDs could serve as the quantum memory in the quantum repeater [2] or as a local entangler to create a photonic state for a memory-free quantum repeater [3].

In this talk, we present our experimental results for electrically contacted charge-tuneable p-i-n InAs QDs embedded in a circular Bragg grating (CBG). The cavity design enables us to control the charged exciton states of the quantum dots. The CBG exhibits high Purcell enhancement in a broad wavelength range. A novel labyrinth design of the CBG allows for electrical contacting without impeding other performance characteristics [4].

[1] D. Vajner et al., Adv. Quantum Technol. (2022), 10.1002/qute.202100116 [2] H.-J. Briegel, W. Dür, J. I. Cirac and P. Zoller, Phys. Rev. Lett. 81, 5932*5935 (1998), 10.1103/PhysRevLett.81.5932 [3] K. Azuma, K. Tamaki and H.-K. Lo, Nature communications 6, 6787 (2015)., 10.1038/ncomms7787 [4] Q. Buchinger et al., Appl. Physics Letters (2023), 10.1063/5.0136715

HL 37: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)

The session is the first part of the focus session on the physics of the van der Waals magnetic semiconductor CrSBr, with a main session on Friday morning. The focus session is jointly organized by HL and MA.

Time: Wednesday 15:00–15:30 Location: H15

HL 37.1 Wed 15:00 H15

Doping-control of excitons and magnetism in few-layer CrSBr — •Farsane Tabataba-Vakili[1,2,3], Anna Rupp[2], Huy Nguyen[2], Anvar Baimuratov[2], and Alexander Högele[2,3] — [1]Institute of Condensed Matter Physics, Technische Universität Braunschweig, Braunschweig, Germany — [2]Fakultät für Physik, Munich Quantum Center, and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, München, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

In two-dimensional (2D) magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-layer CrI3. Within the class of 2D magnets, air-stable CrSBr stands out as an antiferromagnetic semiconductor with a high Néel temperature, excitons coupled to the magnetic order, and exciton-magnon coupling. In this talk, I will present our work on doping-control of excitons and magnetism in few-layer CrSBr [1]. We demonstrate that both exciton and magnetic transitions are sensitive to field-effect charging, exhibiting bound exciton-charge complexes and doping-induced metamagnetic transitions. We further visualize magnetic domain formation induced by magnetic field or charge-doping at the metamagnetic transition all-optically by raster-scan reflectance imaging. Our work identifies few-layer CrSBr as a rich platform for exploring collaborative effects of charge, optical excitations, and magnetism.

[1] F. Tabataba-Vakili et al., Nat. Commun. 15, 4735 (2024).

HL 37.2 Wed 15:15 H15

Proximity-Induced Exchange Interaction and Prolonged Valley Lifetime in $MoSe_2$/CrSBr Van-Der-Waals Heterostructure with Orthogonal Spin Textures — •Andreas Beer[1], Klaus Zollner[1], Caique Serati de Brito[1,2], Paulo E. Feria Junior[1], Philipp Parzefall[1], Talieh S. Ghiasi[3], Josep Ingla Aynés[3], Samuel Mañas-Valero[4], Carla Boix-Constant[4], Kenji Watanabe[5], Takashi Taniguchi[5], Jaroslav Fabian[1], Herre S. J. van der Zant[3], Yara Galvão Gobato[2], and Christian Schüller[1] — [1]UR, Regensburg, Germany — [2]UFSCar, São Carlos, Brazil — [3]TU, Delft, Netherlands — [4]ICMol, València, Spain — [5]NIMSC, Tsukuba, Japan

We report a comprehensive optical study of a ML-$MoSe_2$ on the layered A-type antiferromagnetic semiconductor CrSBr. The band alignment of the material combination is under debate. Here, we adopt the type-III band alignment picture. By performing co-circular polarized PL and reflection contrast (RC) experiments, we observe that the atomic proximity of the materials leads to an unexpected breaking of time-reversal symmetry, despite the originally perpendicular spin texture in both materials, which are further supported by first-principles calculations. Moreover, time-resolved PL and time-resolved RC measurements identify a very long-lived dynamic charge-transfer process in the heterostructure, consistent with a type-III band alignment. Our findings suggest band bending, and efficient Förster resonance energy transfer within the heterostructure. Finally time resolved Kerr ellipticity measurements reveal a two magnitudes prolonged valley lifetime.

HL 38: Nanomechanical systems (joint session HL/TT)

The session covers the physics of nanomechanical systems.

Time: Wednesday 15:00–15:45 Location: H17

HL 38.1 Wed 15:00 H17

Optimizing an Integrated Photonic Racetrack Resonator for Optomechanical Synchronization — •Agnes Zinth[1] and Menno Poot[1,2,3] — [1]Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Institute for Advanced Study, Technical University of Munich, Garching, Germany

In the field of optomechanics, synchronization will be an essential tool in fields like sensing and quantum technologies. Towards this goal, we develop a photonic integrated optomechanical device consisting of a silicon nitride racetrack cavity with partly suspended waveguide that can vibrate freely. A second beam is added to improve the optomechanical coupling. The observed mechanical modes do not match in frequency, so we use a predisplaced beam instead [1]. The remaining frequency distance can be tuned by the laser power. As the light propagates in the predisplaced beam and only past the PhC beam, it shifts further than the photonic crystal one due to thermal effects. To synchronize them with optomechanical backaction, we also need to enhance the optical cavity. Therefore, we modify the transition from supported to suspended parts. Two different approaches lead to the desired improved optical quality. Currently, we are investigating their impact on the mechanics. We believe that, in the next generation of devices, we can synchronize the racetrack and photonic crystal beam.

[1] Geometric tuning of stress in predisplaced silicon nitride resonators. Nano Letters, 22(10), 4013-4019.

HL 38.2 Wed 15:15 H17

Quantum Mechanics in Two-Dimensional Dynamic Spaces — •Benjamin Schwager and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

In the study of systems with reduced dimensions one encounters quantum particles under spatial constraints. Their dynamics have to be modeled based on a configuration space that is a Riemannian manifold, in general, and the resulting quantum wave equations contain correction terms in dependence of its geometric properties. We consider particles which are confined to a flexible thin material shell by studying the Schrödinger equation on moving domains. The model assumes a static observer and couples the deformation dynamics of the material to the quantum dynamics it hosts via additional potential fields. Effects caused by the interplay of geometry and the temporal evolution of the underlying configuration space will be discussed.

HL 38.3 Wed 15:30 H17

Towards cavity optomechanics using 2D materials — •Petricia Sara Peter[1,2], Lukas Schleicher[1,2], Anne Rodriguez[1,2], Leonard Geilen[2,3], Alexander Musta[2,3], Benedict Brouwer[2,3], Alexander Holleitner[2,3], and Eva Weig[1,2] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Walter Schottky Institute, TU Munich, Germany

Two-dimensional (2D) materials, such as hexagonal boron nitride (hBN), are promising candidates for advancing cavity optomechanics due to their low mass, high mechanical strength, and unique optical properties. This work focuses on the fabrication of freely suspended hBN membranes on silicon oxide (SiO_2) and silicon nitride (Si_3N_3) substrates, utilizing a water-assisted wet transfer technique. Compared to the dry transfer method, this approach minimizes inhomogeneous stress and preserves optimal mode shapes, improving mechanical quality factors. A Michelson interferometer is used to measure the mechanical properties of the resulting drumhead resonators, including vibrational resonances, mode shapes, and quality factors. These results provide important insights into the performance and quality of the resonator, laying the groundwork for incorporating 2D materials into cavity optomechanical studies.

HL 39: Poster III

The third poster session covers most recent results on the optical and thermal properties of semiconductors, as well as on nitrides and organic semiconductors, and semiconductor lasers.

Time: Wednesday 15:00–18:00 Location: P3

HL 39.1 Wed 15:00 P3

Termperature dependent electroluminescence spectroscopy of far-UVC-LEDs with varying AlGaN quantum well thickness — •Max Dittmer[1], Jakob Höpfner[1], Markus Blonski[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[2], Sven Einfeldt[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1] — [1]TU Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Insitut (FBH), Berlin Germany

AlGaN far-UVC-LEDs with emission wavelengths below 240 nm require AlGaN layers with such high aluminium molefractions that p-doping with magnesium is inefficient due to its high ionization energy. An alternative method of p-doping is distributed polarization doping (DPD), which induces charge carriers by polarization charges. We will present the results of temperature dependent electroluminescence spectrocopy on 233 nm AlGaN LEDs with DPD gradient, grown by metal organic vapor phase epitaxy (MOVPE). We investigated the impact of the quantum well (QW) width from 1.3 nm to 7.6 nm. Most importantly we found the 2.6 nm LED to be the most efficient at room temperature. The LEDs exhibit an S-shape in the emission energy in dependence of the temperature and the highest internal quantum efficiency of 55%, was measured at 200 K.

HL 39.2 Wed 15:00 P3

MATRIX: GaN diode arrays for proton monitoring and imaging — •Nico Brosda[1], Stéphane Higueret[2], Thê-Duc Lê[2], Andreas Wieck[1], Maxime Hugues[3], Matilde Siviero[3], and Jean-Yves Duboz[3] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Université de Strasbourg, CNRS, IPHC UMR 7178, F-67000 Strasbourg, France — [3]Université Côte d'Azur, CNRS, CRHEA, 06560, Valbonne, France

The MATRIX project is pioneering advancements in proton therapy for cancer treatment by developing novel, highly durable detectors that enhance real-time control of irradiation doses. Proton detection is achieved by measuring the current induced in the active regions of PIN GaN diodes. Our GaN-based devices are fabricated as linear diode arrays of 128 elements and two-dimensional imaging arrays up to 11×11 elements, covering an area of 1 cm^2 with up to 500 μm spatial resolution. Thanks to the microelectronics processes, a much higher resolution can be obtained if needed. Results concerning the sample structure and fabrication process are presented. The design of bonding contacts proved to have a significant impact on the measured signal and, thus, the imaging quality. A bonding fanout on the GaN samples introduced notable signal distortions at the edges of the proton irradiation field. The underlying electron external emission mechanism responsible for this distortion was modeled, and a correction method was developed. An adapted sample design improved the device quality and removed the signal distortion. These findings pave the way for optimizing future GaN-based proton detector arrays.

HL 39.3 Wed 15:00 P3

Investigating the Electrical Properties of Distributed Polarization Doped $Al_xGa_{1-x}N$ Heterostructures via Capacitance-Voltage Measurements — •Thibaut Ehlermann[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim

Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin — [2]Ferdinand-Braun-Institut (FBH)

Distributed Polarization Doping (DPD) enables the generation of charge carriers in wide-bandgap semiconductors like AlGaN by utilizing the material's inherent polarization properties without the introduction of impurities. Linearly graded AlGaN DPD layers were grown by metal-organic vapor phase epitaxy (MOVPE). The starting Al mole fraction was always 100%. The thickness and end mole fraction were varied. The charge carrier concentration N_A was determined from CV-measurements. For a 100 nm thick AlGaN DPD layer (x=100% –> 60%), the charge carrier concentration is $N_A = 1.4 \cdot 10^{18} \frac{1}{\mathrm{cm}^3}$, closely matching the theoretical value of $N_A = 1.72 \cdot 10^{18} \frac{1}{\mathrm{cm}^3}$, based on the calculated intrinsic polarization. Thicker DPD layers lead to a lower doping concentration and AlGaN DPDs (x=100% –> 80%) result in lower doping concentrations in agreement with the calculated values. The consistency of the results suggest that DPD is a reliable and promising way for p-type doping in AlGaN.

HL 39.4 Wed 15:00 P3

Temperature Dependence of the Quantum Efficiency of UV LEDs emitting from 226 nm to 300 nm — •Max Eysell[1], Jakob Höpfner[1], Marcel Schilling[1], Norman Susilo[1], Anton Muhin[1], Massimo Grigoletto[1,2], Tim Kolbe[2], Arne Knauer[2], Sylvia Hagedorn[2], Markus Weyers[2], Jens Rass[2], Hyun Kyong Cho[2], Tim Wernicke[1], Sven Einfeldt[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

UV-LEDs are of huge interest for e.g. air, surface, and water disinfection. However, the widespread application of UV-LEDs is constrained by their external quantum efficiency (EQE) which is decreasing further as the emission wavelength shortens. To gain insight into the carrier transport and recombination mechanisms, a detailed analysis of the EQE of UV-LEDs and the three contributors: the carrier injection, the radiative recombination and the light extraction was performed.

The emission power of LEDs with emission wavelengths of 226 nm, 233 nm, 265 nm and 305 nm are investigated by temperature dependent electroluminescence measurements in the range of $25 - 80°C$. A reduction in emission power and EQE has been observed going from UVB to the far-UVC spectral range. A thermal droop in the emission power was observed for all samples which is caused by the decline of all three contributions. The magnitude of this thermal droop becomes higher with decreasing wavelength which we attribute to an increased electron leakage suggested by Schrödinger-Poisson drift-diffusion simulations.

HL 39.5 Wed 15:00 P3

Theoretical Study on the (In, Ga)N/GaN heterojunction — •Maximilian Lauer[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Semiconductor materials have a wide range of applications and their electronic properties can be easily tuned by alloying and changing their composition x. Understanding the properties of semiconductor alloys, such as indium gallium nitride $In_xGa_{1-x}N$, is therefore an important area of research. Two such properties are the band gap of the semiconductor and its band alignment with substrate and conduction materials.

While the band gap of the random alloy (In, Ga)N is a well-established quantity, the band alignment is less well understood.

Our research aims to better understand the band alignment and interface states at a GaN/(Ga,In)N heterojunction and its impact on the electronic properties of the system.To achieve this, we performed DFT calculations using the Korringa-Kohn-Rostoker (KKR) formalism with the coherent potential approximation (CPA). From these calculations we computed the layer-resolved density of states (DOS) for varying $In_xGa_{1-x}N$ compositions. This approach can be further used to simulate the effects of doping on the electronic properties or to study the transport properties of such a system.

HL 39.6 Wed 15:00 P3

Moiré exciton polaritons in twisted photonic lattices at room temperature — •Tobias Schneider[1], Chunzi Xing[2], Yu Wang[3], Xiaokun Zhai[2], Xinzheng Zhang[3], Haitao Dai[2], Xiao Wang[4], Anlian Pan[4], Zhenyu Xiong[5], Hao Wu[5], Yuan Ren[5], Stefan Schumacher[1,6], Xuekai Ma[1], and Tingge Gao[2] — [1]Physics dept. and CeOPP, Paderborn University, Germany — [2]Department of Physics, School of Science, Tianjin University, Tianjin 300072, China — [3]The MOE Key Laboratory of Weak-Light Nonlinear Photonics and International Sino-Slovenian Join Research Center on Liquid Crystal Photonics, TEDA Institute of Applied Physics and School of Physics, Nankai University, Tianjin 300457, China — [4]College of Materials Science and Engineering, Hunan University, Changsha 410082, China — [5]Lab of quantum detection and awareness, Space Engineering University Beijing 101416, China — [6]PhoQS, Paderborn University, Germany

Due to their support of many exotic physical phenomena such as Mott insulators or the fractal quantum Hall effect, moiré lattices have attracted great interest. In this work, rhombic optical moiré lattices are realized in microcavity exciton polaritons[1]. These lattices consist of two stacked 1D periodically patterned stripes which are twisted to a specific angle. This structure allows the resulting bands to be tuned via modulating the lattice parameters such as the periodicity, the potential depth of the stripes, and the rotation angle. In addition, moiré polaritons in twisted 2D honeycomb lattices are also observed. [1] C. Xing et al., arXiv:2408.02431 (2024).

HL 39.7 Wed 15:00 P3

Ultradoped GeSn plasmonic antennas for IR photodetection — •Guillermo Godoy[1,2], Ali Azimi[3], Fritz Berkmann[3], Oliver Steuer[1], Slawomir Prucnal[1], Shengqiang Zhou[1], Ing-Song Yu[4], Inga A. Fischer[3], and Yonder Berencén[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden Germany — [2]Dresden University of Technology, Dresden Germany — [3]BTU Cottbus-Senftenberg, Cottbus Germany — [4]National Dong Hwa University, Hualien Taiwan

Ligth mater interaction due to localized surface plasmon resonances (LSPRs) can generate hight electical field enhacement, enabling biosensing and hot-electron photodetection devices. While metallic nanoparticles like Au and Al are commonly used, their optical losses increase at longer wavelengths, limiting applications in the mid-infrared (MIR) range, such as air pollution detection. Highly doped group-IV semiconductors, particularly GeSn alloys, offer a cost-effective alternative with lower losses and CMOS compatibility. The cut-off wavelength for plasmonic resonances depends on the carrier effective mass, and GeSn alloys with its lower electron effective mass enables plasmonic resonances from shorter wavelengths.This work explores strategies to achieve highly doped GeSn alloys for plasmon-enhanced photodetection, utilizing MBE or CVD-grown GeSn layers on Si substrates. These layers will be doped in-situ or ex-situ via ion implantation, followed by non-equilibrium annealing to enhance crystal quality and dopant activation, showcasing their potential for advancing MIR photodetection.

HL 39.8 Wed 15:00 P3

Optical and phonon properties of In-rich InGaN alloys and InN/InGaN multiple quantum well structures — •Svitlana Polesya[1], Masako Ogura[1], Sergiy Mankovsky[1], Gregor Koblmüller[2], and Hubert Ebert[1] — [1]University of Munich, 81377 Munich, Germany — [2]Technical University of Munich, 85748 Garching, Germany

In two-dimensional systems like multiple quantum well structures, thermalization of hot carriers can be strongly suppressed. InN/InGaN multilayered (ML) materials are seen as promising candidates to show this property. In order to optimize these materials, ab initio calculations have been performed on the electronic and phonon band structure, as well as on the optical properties of In-rich $In_xGa_{(1-x)}N$ alloys and the short period ML systems $[InN]_m/[In_xGa_{(1-x)}N]_n$. All calculations have been done with the VASP package. The HSE exchange-correlation potential has been used with further GW0 corrections. Electron-hole interactions were taken into account by solving the Bethe-Salpeter equation. The calculations on alloys were done via the superlattice technique considering for each In concentration x all non-equivalent atomic arrangements. This is crucial as the atomic distribution has a significant impact on the phonon band structure of the alloys. For the layered $[InN]_m/[In_xGa_{(1-x)}N]_n$ system the optical properties were calculated for various concentrations x. The important role of the interface between the quantum well ($[InN]_m$) and the quantum barrier ($[In_xGa_{(1-x)}N]_n$) on the optical properties as well as phonon band gap is shown.

HL 39.9 Wed 15:00 P3

Ultra-sensitive absorption measurements of perovskites nanocrystals, protein crystals and photo-switchable lipids — •Ayesha Khan[1], Simone Strohmair[1], Ines Amersdorffer[1,2], David Hunger[3], and Thomas Hümmer[1,2] — [1]Qlibri GmbH, Munich, Germany — [2]Ludwig Maximilian University of Munich, Munich,

Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Optical studies of nano-scale systems through spectroscopy and imaging can reveal intrinsic optical properties of materials including resolving the exitonic fine structure of systems. However, due to diminutive absorption of nano-scale systems, it is challenging to perform absorption spectroscopy. For a nano-scale system placed inside an optical resonator, the light passes through the sample thousands of times, enhancing the absorption and thus, allowing measurements.

Here we present the use of a fiber-based, open-access micro-cavity to image and obtain hyperspectral maps of absorption for different nano-scale, solid state materials including perovskites nanocrystals, protein crystals and photo-switchable lipids.

The successful measurements of different nano-scale systems promise that fiber-based microcavities can become standard tools for absorption measurements of these systems.

HL 39.10 Wed 15:00 P3

Intensity-dependence of the excitonic third-harmonic generation in bilayer MoS2 — •Ruixin Zuo[1], Matthias Reichelt[1], Cong Ngo[1], Xiaohong Song[2], and Torsten Meier[1] — [1]Department of Physics, Paderborn University, D-33098 Paderborn, Germany — [2]School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570288, China

The large exciton binding energies make layered transition metal dichalcogenides an ideal platform for exploring exciton physics in two-dimensional systems. We numerically and theoretically investigate three-photon transitions to the excitonic states in a bilayer MoS2 and demonstrate that beyond the linear order intraband transitions dominate over interband transitions. Beyond the perturbative limit, transitions to and from the continuum that represent fifth- and higher-order nonlinearities contribute to the excitonic response at the third harmonic where they destructively interfere with the third-order excitations. Applying an in-plane static electric field characteristically modifies the k-resolved fourth-order and higher-order nonlinearities and accordingly the interference at the excitonic resonance. We demonstrate that the yield of the third harmonic generation may rise with increasing static field strength. This finding can be interpreted to arise from a shift from destructive to constructive interference between the lowest- and higher-order excitations. Exciton ionization prevails at even higher static field strengths and results in a decrease of the third harmonic generation.

HL 39.11 Wed 15:00 P3

Implementation and Validation of a Herzberg-Teller Approach for Phonon-Assisted Photoluminescence — •Tobias Dittmann, Torben Steenbock, and Gabriel Bester — Insitut für physikalische Chemie, Universität Hamburg

Phonon-assisted PL from electronically excited states leads to the occurrence of phonon side-bands, which can shape the PL spectrum. A Franck-Condon framework based on Huang-Rhys factors efficiently describes phonon side-bands in nanostructures containing up to a few hundred atoms.[1] However, the FC approximation is usually not suited for the emission from a dark state. Therefore, we extend the method towards a Herzberg-Teller (HT) level which allows a more accurate description of the emission from a dark state. Additionally, our method includes the description of spin-orbit effects, offering an advantage over other implementations of the HT framework, particularly for structures containing heavy elements.

In a first stage of the project, we investigate various graphene quantum dots and observe that the inclusion of HT terms introduces both quantitative and qualitative differences compared to the FC spectrum. These findings underscore the critical importance of incorporating HT terms for accurate modelling. In future work, we intend to apply this method to bigger structures containing heavy elements, in order to benefit from the advantages of our implementation.

[1] Wu, Han, Dittmann, Wang, Zhang and Bester, Nanoscale, 2024, DOI: 10.1039/D4NR02458C

HL 39.12 Wed 15:00 P3

Electronic structure and energy landscape of $B_{Si}Si_i$-related defects — Aaron Flötotto[1], Wichard Beenken[1], Kevin Lauer[1,2], Stefan Krischok[1], and •Erich Runge[1] — [1]Technische Universität Ilmenau, Institute for Physics, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is an important dopant for silicon. Together with an adjacent interstitial Si atom, it forms the so-called $B_{Si}Si_i$ defect, which has been proposed as a source of light-induced degradation (LID) in solar cells made from boron-doped Czochralski-grown silicon. Furthermore, the $B_{Si}Si_i$ defect is an intermediate configuration in many models for boron diffusion in silicon.

In a recent comprehensive density-functional-theory-based study [1], we have calculated the energy landscape around the $B_{Si}Si_i$ defect and related defects involving one B atom and one interstitial Si atom for different chemical potentials of electrons corresponding to neutral, positively, and negatively charged supercells. Among the found metastable defect configurations, we identify possible recombination centers based on the defect-dependent electronic density of states and the minimal energy paths between them. The resulting potential energy landscape is checked against empirical models for boron diffusion and LID.

[1] A. Flötotto et al., Phys. Rev. Mater. (accepted)

HL 39.13 Wed 15:00 P3

Origin of strong interband transitions in antimony — •Julia Vehndel, Nils Holle, Sebastian Walfort, and Martin Salinga — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, phase change materials (PCMs) have attracted considerable interest as photonic memory elements due to a high contrast in optical properties between crystalline and amorphous states. In order to identify ideal PCMs for specific applications, the intricate connection between electronic structure, bonding and permittivity needs to be understood.

Here, we employ ab-initio simulations based on density functional theory to calculate the optical properties of the single-elemental PCM antimony in the visible and near-infrared. We analyze the permittivity in k-space for both crystalline and amorphous states. Most strikingly, the strong interband transitions at lower energies can be related to the electron and hole pockets in the first Brillouin zone of the crystalline state.

HL 39.14 Wed 15:00 P3

Optical properties of α-$(Cr_xGa_{1-x})_2O_3$ — •Dmitry Sayenko, Clemens Petersen, Jakob Seifert, Christiane Dethloff, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

Due to its high bandgap energy in the order of $4.6-5.0\,\mathrm{eV}$ and its high predicted electrical breakdown field of about $8\,\mathrm{MV\,cm^{-1}}$, Ga_2O_3 is a promising material for transparent electronic devices and high power applications [1]. Of special interest is the corundum-structured α-phase as it has the largest band gap energy of the Ga2O3 polymorphs. Further, its band gap energy can be tuned by alloying with Cr without changing its crystal structure. Here we present the dielectric function of α-$(Cr_xGa_{1-x})_2O_3$ as a function of the cation composition. The sample was grown by combinatorial pulsed laser deposition. As expected, the onset of absorption increases with increasing Ga concentration from around $3.2\,\mathrm{eV}$ for $x \approx 0.74$ to $4.2\,\mathrm{eV}$ for $x \approx 0.13$. Whereas we observe for all concentrations a negative birefringence in the visible range, i.e. $n_{\mathrm{eo}} < n_{\mathrm{o}}$, the polarization of the energetically lowest transition changes with Cr concentration. For large Cr concentration the absorption sets in at first for light polarized perpendicular to the c-axis whereas for large Ga concentration the first absorption is observed for light parallel to the c-axis. This change of the polarizability leads to a decrease of the birefringence with decreasing Cr concentration, but $n_{\mathrm{eo}} < n_{\mathrm{o}}$ holds for all x.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

HL 39.15 Wed 15:00 P3

Calibration methods in Raman spectroscopy — •Susanne Moritz, Ron Hildebrandt, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

For low symmetry materials, polarization resolved measurements are required for a precise investigation, especially of the Raman tensor [1, 2]. Here we present strategies for calibrating and determining the polarization state of the incident and scattered light. In addition to the polarizing optics, e.g. polarizers, we also consider the impact of all involved optical elements such as mirrors and beam splitters. We show, that these non-idealities can have an impact on the determined Raman tensor elements. Taken into account the non-idealities of the polarizing optics the uncertainty of the deduced tensor elements can be reduced by 20%.

[1] C. Kranert *et al.*, Phys. Rev. Lett. **116**, 127401 (2016).
[2] C. Kranert *et al.*, Sci. Rep. **6**, 35964 (2016).

HL 39.16 Wed 15:00 P3

Spectral Signatures and Kinetics of Y6 Aggregates and Disordered Phase via Absorption Spectroscopy — •Daniel Kroh[1,2], Xinyue Xu[2], Trevor Smith[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, EPII, Universität Bayreuth, Bayreuth, Germany — [2]School of Chemistry, University of Melbourne, Melbourne, Australia

Recent advancements in single-junction organic solar cells (OSCs) utilizing non-fullerene acceptors (NFAs) have significantly increased power conversion efficiencies (PCEs) to over 19%. This remarkable progress is largely attributed to the introduction of the "Y-series" NFAs, with Y6 being the most notable example. Motivated by these achievements, numerous research groups are investigating the relationship between film morphologies and their exceptional optoelectronic properties, especially when blended with the donor material PM6.

In our study, we employed temperature-dependent steady-state UV-Vis absorption and photoluminescence spectroscopy combined with Franck-Condon analysis to identify the spectral signatures of two types of aggregates and the disordered phase of Y6 in solution. We observed that all three phases are also present in neat Y6 films and blend films with PM6. Through transient absorption measurements, we further explored the excitation kinetics and transient absorption spectral signatures of these phases, providing deeper insights into their behavior.

HL 39.17 Wed 15:00 P3

Empowering Thermoelectric Performance of ZnSb via Bonding Interaction Regulation — •Meng Jiang[1,2], Fangyi Hu[1], Qihao Zhang[2], Lianjun Wang[2], Wan Jiang[2], Matthias Wuttig[1], and Yuan Yu[1] — [1]Physical Institute 1, RWTH Aachen University, Aachen, 52074, Germany. — [2]Donghua University, Shanghai, 201620, China.

ZnSb compounds have garnered significant attention due to its green nature, low cost and high Seebeck coefficient. However, its thermoelectric performance has been limited by a relatively low power factor and high lattice thermal conductivity. Recent studies have demonstrated that regulating bonding interactions offers an effective strategy to optimize the thermoelectric properties. Specifically, metavalent bonding shows unprecedented success in predicting and optimizing a series of high-performance thermoelectric materials. This reignites research interest in ZnSb. We explored a one-step synthesis strategy for ZnSb and specifically investigated optimizing mechanisms of Cd and Mg. By regulating bonding interactions to optimize electrical conductivity, the room-temperature power factor was enhanced from 2.5 to 4 μW cm-1 K-2. This improvement, coupled with a reduction in lattice thermal conductivity, resulted in a zT of 0.6 at 600 K. Our work highlights the potential of bonding interaction regulation as an effective approach for enhancing the thermoelectric performance of ZnSb. More, future research would focus on unraveling the intricate mechanisms linking bonding and microstructure to achieve even higher performance.

HL 39.18 Wed 15:00 P3

Challenges and Opportunities for Thermoelectric Coolers — •Fangyi Hu, Meng Jiang, Matthias Wuttig, and Yuan Yu — I. Physikalisches Institut (IA), RWTH Aachen University, 52074 Aachen, Germany

Thermoelectric (TE) materials allow a direct interconversion between heat and electricity, providing an eco-friendly and sustainable energy solution. Particularly, thermoelectric coolers based on the Peltier effect achieve high-precision temperature control without any refrigerant. Bi2Te3-based materials have beenused in commercial TE cooling due to their high near-room-temperature figure-or-merit (ZT). Yet, the low earth abundance of Te restricts the large-scale application of this compound. Discovering Te-free materials with comparable cooling performance is an urgent task. This requires a small bandgap and low thermal conductivity for the material at low temperatures. The recently developed concept of metavalent bonding provides a new avenue for discovering potential candidates. Besides materials, the device design and effective heat dissipation on the hot side are of critical importance. This Poster will summarize the challenges and opportunities for TE cooling materials and devices. We hope that it can shed light on the development of new TE coolers.

HL 39.19 Wed 15:00 P3

Quantum-chemical calculations of structure, electronic properties, and spectra of a model for PBDB-T:ITIC heterojunctions — Montassar Chaabani[1], Samir Romdhane[2], and •Wichard J. D. Beenken[2] — [1]Advanced Materials and Quantum Phenomena Laboratory, Physics Department, Faculty of Sciences of Tunis, University of Tunis El Manar, Tuins, Tunesia — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We modeled PBDB-T:ITIC heterojunctions by applying DFT on dimers built of various conformers of a PBDB-T segment and the ITIC molecule. These variations represented the non-uniformity of the interface between the donor and the acceptor in the organic solar cell. Based on this model, we calculated electronic and optical properties most relevant for charge separation at the interface using DFT and TD-DFT, respectively. For almost half of our modeled dimers, we found that the band offsets between them and the pristine donor and acceptor materials resulted in charge carrier trapping leading to inefficient charge separation as well as non-geminate recombination. When we calculated the exciton binding energy by TD-DFT using either the B3LYP or the HSE06 functional, we obtained very different qualitative and quantitative results. We, therefore, compared our results with experimental data from ultraviolet photoelectron spectroscopy, CV, ER-EIS, PL, absorption spectroscopy, EQE and EL. Finally we discuss the impact of our findings on characteristic photovoltaic parameters, particularly the open circuit voltage and the short-circuit current.

HL 39.20 Wed 15:00 P3

Investigation of the optical coupling of lasing ZnO nanowires — •Ann-Kathrin Kollak, Lukas Raam Jäger, Francesco Vitale, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Semiconductor nanowires offer potential for miniaturizing optical circuits. Good candidates for this application are ZnO nanowires, because their bottom-up growth via the Vapor-Liquid-Solid (VLS) mechanism allows for high quality crystal structures. When optically pumped, ZnO nanowires simultaneously act as an active medium and a laser cavity, emitting UV light mainly waveguided to their end facets. To study the interaction of these nanometer-scale lasers via evanescent field coupling, two nanowires were positioned in contact next to each other on a SiO_2 substrate using a nanomanipulator. In a micro-PL (photoluminescence) setup, the nanowire pair was optically excited using the third harmonic of an Nd:YAG laser (355 nm). The pair's emission was collected with the same setup, allowing the investigation of the spatially resolved PL and lasing spectra, as well as their linear polarization parallel to the substrate. The data obtained indicate that ZnO nanowire cavities can couple with one another. Depending on the geometry of the nanowire pair and the pumping conditions, optical modes that extend into both cavities can appear in addition to modes confined to only one nanowire. In other cases, the coupled modes dominate the lasing behavior.

HL 39.21 Wed 15:00 P3

Impact of stress current on reverse-bias electroluminescence images of 850 nm oxide-confined VCSELs — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Sebastian Haberkern[1], Helmut Meinert[1], Alexander Moll[1], Ilya E. Titkov[2], Oleg Yu. Makarov[2], and Nikolay N. Ledentsov[2] — [1]Esslingen University of Applied Sciences, Flandernstrasse 101, 73732 Esslingen, Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Germany

Vertical-cavity surface-emitting lasers (VCSEL) employing different doping of the cavity region are studied utilizing reverse current-voltage (IV) characteristics as well as reverse bias electroluminescence (ReBEL). Reverse IV characteristics exhibits avalanche breakdown enabling an estimation of the electric field in the cavity region. ReBEL emission is observed at locations where avalanche breakthrough current has its maximum. The oxide-confined VCSELs are characterised before and after high current operation. Virgin devices have a homogeneous device center in ReBEL images. Upon a short high current burn-in VCSELs evolved a homogeneous ring at the oxide-aperture perimeter. This ring structure decays into 2 point-like areas after long-term current stress. These observations in ReBEL images can be understood in terms of recently published VCSEL simulation results which gave evidence of local current crowding at the oxide-aperture during high current laser operation.

HL 39.22 Wed 15:00 P3

Tuning nanowire lasers via hybridization with organic molecules — •Philipp Swatosch, Edwin Eobaldt, Marco Grünewald, Olga Ustimenko, Kalina Peneva, and Carsten Ronning — Friedrich Schiller Universität Jena, Deutschland

Among the numerous nanomaterials, semiconductor nanowires have drawn significant scientific interest as promising candidates for nanoscale coherent light sources and all-optical circuits. This attention is due to their exceptional waveguiding properties and inherent ability to lase under high excitation. However, precise control over their lasing characteristics, such as emission wavelength and lasing threshold, is essential for various applications. In this regard, hybridizing nanowires with customized molecules presents a potential approach, providing new control mechanisms through efficient charge and energy transfer processes at the heterointerface. To demonstrate this concept, we hybridized ZnO nanowires with perylene-based organic dyes. These chromophores are particularly advantageous as their optical gap can be easily tuned over a wide spectral range through chemical functionalization. This study employs comparative micro-photoluminescence measurements to investigate the impact of these molecules on the lasing properties of the nanowires.

HL 39.23 Wed 15:00 P3

Development of a VCSEL-chip in the red spectral range with integrated photodiode for chlorophyll fluorescence analysis — •Raphael Buffler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum-Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Chlorophyll fluorescence analysis provides information on photosynthetic activity of plants and thus also on their health. Changes in the environmental conditions can be monitored on large scale and, water and nutrients can be added as needed. In order to induce the fluorescence of chlorophyll in the range from 660 nm to 750nm , optical excitation at 650 nm can be used. In this work, a semiconductor chip will be developed that contains both, the light source for excitation and the photodiode for fluorescence detection. The chip is based on the AlGaAs & AlGaInP material systems, which can realise the band gaps for the required wavelengths. The light source is designed as a vertical-cavity surface-emitting laser (VCSEL), which allows for the vertical emission of the excitation light and the vertical irradiation of the photodiode. A stacked arrangement is used, where the VCSEL is grown by metal-organic vapor-phase epitaxy (MOVPE) on top of the photodiode structure on a GaAs wafer. First electro-optical characteristics of the VCSEL and the photodiode such as P-U-I curves, emission wavelength and photodiode responsivity are presented.

HL 39.24 Wed 15:00 P3

Monolithic 850 nm VCSEL array for Quantum Key Distribution via the Decoy State Protocol — •Katharina Dahler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The need for secure data communication has increased in recent years. In contrast to classical key distribution, the use of quantum key distribution (QKD) offers fundamental advantages, such as complete secrecy. However, QKD poses numerous challenges regarding the use of single photons. With this in mind, the decoy-state protocol offers the possibility of realizing QKD with classical light sources such as attenuated semiconductor lasers. Here, we present the electro-optical characterization of a monolithic 850 nm vertical-cavity surface-emitting laser (VCSEL) array, for QKD via the BB84 and decoy state protocol. The complete VCSEL array consists of eight individual VCSELs arranged in a coplanar contact design, with four VCSELs serving as signal states and four as decoy states. A highly homogeneous growth is needed due to the requirement of indistinguishable light pulses regarding the emission wavelength. In order to realize the four necessary polarization states and to counteract the electro-optical effect, each VCSEL features a monolithically integrated surface grating in the top layer of its light emission window. Electro-optical device characteristics regarding light polarization via surface gratings and spectral homogeneity of the VCSEL array are presented.

HL 39.25 Wed 15:00 P3

A machine learning potential for tellurium — •Andrea Corradini, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Elemental tellurium has drawn attention in recent years, due to its possible technological application as switching device in phase change memories [1]. Recent computational studies are addressing the behaviour of elemental Te under operating conditions with a focus on the crystallization dynamics [2]. In addition, experiments have found anomalous thermodynamic maxima in undercooled liquid Te around 615 K, i.e. 130 K below the melting point [3]. Thermodynamic maxima behave in a very similar way as those in undercooled liquid water. Hence the question whether elemental Te shows a liquid-liquid phase transition, analogously to what is claimed for water. In this work, we develop a robust machine learning potential to study elemental Te and try to answer this question.

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[1] Shen et al., Science 374, 1390*1394 (2021)
[2] Zhou et al., arXiv:2409.03860 [cond-mat.mtrl-sci]
[3] Sun et al., PNAS 119 (28), e2202044119 (2022)

HL 40: 2D Semiconductors and van der Waals Heterostructures IV

The session covers the magnetic and topological properties of 2D semiconductors and van der Waals heterostructures.

Time: Wednesday 15:30–19:00 Location: H15

HL 40.1 Wed 15:30 H15

Dielectric tensor of the layered magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Sebastian Schaper[1], Marie-Christin Heissenbüttel[1], Aleksandra Lopion[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

Two-dimensional materials exhibit unique properties due to their atomically thin structure and weak van der Waals (vdW) coupling between layers resulting in layer dependent properties. As in the case of the layered magnetic semiconductor CrSBr, individual layers are ferromagnetically ordered below the Neel temperature (TN= 132K), while adjacent layers are coupled antiferromagnetically. Due to the highly anisotropic electronic bands in CrSBr, electronic and excitonic states at the fundamental band-gap behave quasi-one-dimensional [1]. To develop a better understanding of the extraordinary light-matter interaction in CrSBr, we access the materials dielectric tensor in the paramagnetic phase by spectroscopic imaging ellipsometry that is hard to access by alternative approaches such as reflectance measurements due to the strong anisotropy. In agreement with theory, we extract highly anisotropic dielectric functions along the crystallographic main axes with strong excitonic resonances particularly in the plane. [1] J. Klein et al. ACS Nano, 17, 6, 5316-5328 (2023).

HL 40.2 Wed 15:45 H15

Raman Polarization Switching in CrSBr — •Priyanka Mondal[1], Daria I. Markina[1], Lennard Hopf[1], Lukas Krelle[1], Sai Shradha[1], Julian Klein[2], Mikhail M. Glazov[3], Iann Gerber[4], Kevin Hagmann[1], Regine v. Klitzing[1], Kseniia Mosina[5], Zdenek Sofer[5], and Bernhard Urbaszek[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Massachusetts Institute of Technology, Cambridge, United States — [3]St. Petersburg, Russia — [4]Université de Toulouse,Toulouse, France — [5]University of Chemistry and Technology, Prague,Czech Republic

Semiconducting CrSBr is a layered A-type antiferromagnet, with individual layers antiferromagnetically coupled along the stacking direction. Due to its unique orthorhombic crystal structure, CrSBr exhibits highly anisotropic mechanical and optoelectronic properties acting it-

self as a quasi-1D material. CrSBr demonstrates complex coupling phenomena involving phonons, excitons, magnons, and polaritons. Here we show through polarization-resolved resonant Raman scattering the intricate interaction between the vibrational and electronic properties of CrSBr. For samples spanning from few-layer to bulk thickness, we observe that the polarization of the A_g^2 Raman mode can be rotated by 90 degrees, shifting from alignment with the crystallographic a (intermediate magnetic) axis to the b (easy magnetic) axis, depending on the excitation energy. In contrast, the A_g^1 and A_g^3 modes consistently remain polarized along the b axis, regardless of the laser energy used. We access real and imaginary parts of the Raman tensor in our analysis, uncovering resonant electron-phonon coupling.

HL 40.3 Wed 16:00 H15

Resonant Inelastic Light Scattering on CrSBr — •Jan-Hendrik Larusch[1], Pierre-Maurice Piel[1], Nicolai-Leonid Bathen[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van der Waals material CrSBr is an optically active semiconductor and an air-stable 2D magnet with ferromagnetic (FM) ordering within each layer and antiferromagnetic (AFM) coupling between adjacent layers, alongside triaxial magnetic anisotropy. Additionally, CrSBr has a highly anisotropic electronic band structure, rendering it a quasi-one-dimensional electronic system, resulting in linearly polarized excitons that are strongly bound [1]. Distinct differences in excitonic emission signatures arise depending on the transition in magnetic ordering from AFM to FM states [2]. To study the coupling between excitons and collective excitations, we employ magnetic field-dependent resonant inelastic light scattering (RILS) experiments at temperatures well below the Néel temperature (˜4K). While first-order phonon modes in Raman spectra remain mostly unaffected by magnetic ordering, RILS reveals resonantly enhanced as well as additional, magnetic field-dependent modes. The later are interpreted as spin-density excitations aka magnon modes. The combined PL and RILS study reveal strong interactions between electronic, excitonic, lattice and spin degrees of freedom. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023) [2] M.C. Heißenbüttel et al. (2024). arXiv:2403.20174.

HL 40.4 Wed 16:15 H15

Disentangling three anisotropic resistivities of the topological insulator α-Bi_4Br_4 — •Jonathan K. Hofmann[1,2], Serhii Kovalchuk[1,3], Yuqi Zhang[4,5,6], Vasily Cherepanov[1], Timofey Balashov[1], Zhiwei Wang[4,5,6], Yugui Yao[4,5,6], Irek Morawski[3], F. Stefan Tautz[1,2], Felix Lüpke[1,7], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Lehrstuhl für Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Institute of Experimental Physics, University of Wrocław, Poland — [4]Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement, Ministry of Education, School of Physics, Beijing Institute of Technology, China — [5]Beijing Key Lab of Nanophotonics and Ultrafine Optoelectronic Systems, Beijing Institute of Technology, China — [6]International Center for Quantum Materials, Beijing Institute of Technology, China — [7]II. Physikalisches Institut, Universität zu Köln, Germany

The higher-order topological insulator α-Bi_4Br_4 is a promising, highly anisotropic quasi one-dimensional van der Waals material. Using a four-tip scanning tunneling microscope, we combine four-point resistance measurements in the square geometry on a bulk sample of α-Bi_4Br_4 with four-point resistance measurements on thin flakes in a linear configuration to disentangle the anisotropic resistivity tensor at room temperature (RT) and at 77 K: At RT, the resistivity along the chain direction is 6.4 times smaller than the resistivity perpendicular to the chains. At 77 K, this anisotropy reduces to 5.0. The vertical anisotropies are $\sim$ 1300 and $\sim$ 6500, at RT and 77 K, respectively.

15 min. break

HL 40.5 Wed 16:45 H15

Spin Hall effect in van-der-Waals ferromagnet — •Tomoharu Ohta[1,2], Nan Jiang[3,4,5], Yasuhiro Niimi[3,4,5], Kohei Yamagami[6], Yoshinori Okadada[6], Yoshichika Otani[7,8], and Kouta Kondou[4,8] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Depertment of Physics, Osaka University, Osaka, Japan — [4]Institute for Open and Transdisciplinary Research Initiatives (OTRI), Osaka, Japan — [5]Center for Spintronics Research Network (CSRN), Osaka, Japan — [6]Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan — [7]Institute for Solid State Physics, The University of Tokyo Chiba, Japan — [8]RIKEN Center for Emergent Matter Science (CEMS), Saitama, Japan

We investigated the spin Hall effect (SHE) in a vdW ferromagnet Fe5GeTe2 (FGT) with a TC of 310 K utilizing the spin torque ferromagnetic resonance method. In synchronization with the emergence of the ferromagnetic phase resulting in the anomalous Hall effect (AHE), a noticeable enhancement in the SHE was observed below TC. On the other hand, the SHE shows a different temperature dependence from the AHE below 120 K: the effective spin Hall conductivity clearly enhanced below TC unlike the anomalous Hall conductivity, might be reflecting variation of band-structure accompanied by the complicated magnetic ordering of the FGT. The results provide a deep understanding of the SHE in magnetic materials to open a new route for novel functionalities in vdW materials-based spintronic devices.

HL 40.6 Wed 17:00 H15

Pseudo-magnetotransport simulations in strained graphene — •Alina Mrenca-Kolasinska[1] and Ming-Hao Liu[2] — [1]AGH University, Krakow, Poland — [2]National Cheng Kung University, Tainan, Taiwan

Graphene, a 2D material consisting of carbon atoms, despite its simple structure and composition can host intriguing phenomena. Application of inhomogeneous strain can lead to pseudomagnetic field (PMF), predicted to have opposite sign in the K and K 0 valley. Special strain profiles have been designed to generate uniform pseudomagnetic field in graphene [1, 2].

In this work we consider transport in pseudo magnetic field in these strain configurations. By deforming the sheet we can control the PMF, and design geometries which allow us to demonstrate interesting transport phenomena. These include electron focusing and snake states observed without external magnetic field present. For efficient modeling of quantum transport within these scenarios in large-scale systems close to realistic size devices, we extend the scalable tight-binding model [3] to accurately capture the effect of displacement field in the Hamiltonian. Our investigations open new possibilities for control over the valley degree of freedom.

[1] F. Guinea, et al., Phys. Rev. B 81, 035408 (2010).

[2] F. Guinea, M. I. Katsnelson, and A. K. Geim, Nat. Phys. 6, 30 (2010).

[3] M.-H. Liu, et al., Phys. Rev. Lett. 114, 036601 (2015).

HL 40.7 Wed 17:15 H15

Strong magnetic proximity effect in van der Waals heterostructures driven by direct hybridization — •Claudia Cardoso[1], Antomio T. Costa[2], Allan H. McDonald[3], and Joaquin Fernandez-Rossier[2] — [1]S3 Centre, Istituto Nanoscienze, CNR, Via Campi 213/a, 41125 Modena, Italy — [2]International Iberian Nanotechnology Laboratory, 4715-330 Braga, Portugal — [3]Physics Department, University of Texas at Austin, Austin, Texas 78712, USA

Proximity effects may induce an electronic property of a material, to an adjacent material in which that property is not present. Here we propose a class of magnetic proximity effects based on the spin-dependent hybridisation. We consider the hybridisation between the electronic states at the Fermi energy in a nonmagnetic conductor and the narrow spin-split bands of a ferromagnetic insulator.

Unlike conventional exchange proximity, this proximity effect has a strong impact on the nonmagnetic layer and can be further modulated by application of an electric field.

Using density functional theory calculations, we illustrate this effect in graphene placed next to a monolayer of CrI_3, a ferromagnetic insulator. The calculations show a strong hybridisation of the graphene bands with the narrow conduction band of CrI_3 in one spin channel only. Furthermore, the results confirm that the hybridisation strength can be modulated by an out-of-plane electric field, paving the way for applications.

HL 40.8 Wed 17:30 H15

Magnetotransport in heterostructures of MBE-grown BS/BSTS and graphene — •Marina Marocko[1], Matthias Kronseder[1], Tobias Rockinger[1], Takashi Taniguchi[2], Kenji Watanabe[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-

0044, Japan

A number of novel phenomena have been observed or predicted in heterostructures of topological insulators and graphene. Similar to transition metal dichalcogenides, topological insulators are expected to dramatically increase the intrinsically very low spin-orbit coupling (SOC) in graphene due to the proximity effect. This opens the way for a range of potential applications, including a spin transistor based on the spin-orbit valve effect.

In our recent experiments, we used a thin MBE-grown film of BS/BSTS topological insulator to induce SOC in graphene. This material has the advantage of adjustable stoichiometry and thus increased possibilities of band structure engineering. The SrTiO3 substrate used for the MBE growth of BS/BSTS also serves as a gate dielectric.

Magnetotransport measurements at 1.7K show a very distinct and narrow weak antilocalization peak around zero magnetic field, which is a sign of induced SOC in graphene. The fitting procedure yields approximate values of the Rashba and valley-Zeeman spin-orbit coupling. We discuss how the extracted SOC values compare with theoretical predictions.

HL 40.9 Wed 17:45 H15

Exploring the valley splitting and valley dynamics of WSe_2 proximity-exchange coupled to CrI_3 — •Natalie Kuhn[1], Marc Schütte[1], Jo Henri Bertram[1], Frank Volmer[1], K. Watanabe[2], T. Taniguchi[3], Christoph Stampfer[1,4], Lutz Waldecker[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Research Centre for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [4]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Proximity exchange coupling between 2D magnets and monolayers of transition metal dichalcogenides (TMDs) can lift valley degeneracy of the TMD. This is promising for the field valleytronics, as valley splitting is expected to increase valley lifetimes.

In this study, we investigate the proximity exchange coupling in van der Waals heterostructures made of monolayer WSe_2 and few-layer CrI_3, a 2D antiferromagnet. The proximity-induced valley splitting of WSe_2 is spatially probed by reflection contrast measurements of WSe_2 excitons. We observe distinctly different regions in WSe_2 identified by their reversed valley splitting. Their origin is explored by their magnetic field dependent reversals, i.e. hysteresis curves that are induced by reversing the magnetization of the interface layer of CrI_3. Using time-resolved Kerr rotation measurements we find a strong enhancement of WSe_2 valley lifetimes of the spin split valence bands.

HL 40.10 Wed 18:00 H15

Excitonic traps in freely suspended 2D membranes — •Alexander Musta[1,3], Leonard Geilen[1,3], Lukas Schleicher[2,3], Benedict Brouwer[1,3], Petricia Sara Peter[2,3], Anne Rodriguez[2,3], Eva Weig[2,3], and Alexander Holleitner[1,3] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Chair of Nano and Quantum Sensors, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

We present studies on the strain profile of large-area suspended transition-metal-dichalcogenides monolayers by photoluminescence measurements. Variations in the strain profile lead to band bending, which results in a redshift of the excitonic spectrum. Additionally, we observe an increase in intensity at the center of the suspended structures. We correlate the excitonic luminescence profiles with mechanical characterizations of the membranes, including AFM measurements and spatial mode mapping.

HL 40.11 Wed 18:15 H15

Rabi Splitting in Quantum Wells and TMDCs: Influence of Many-Particle Coulomb Correlations — •Henry Mittenzwey[1], Felix Schäfer[2], Markus Stein[2], Oliver Voigt[1], Lara Greten[1], Daniel Anders[2], Isabel Müller[2], Florian Dobener[2], Marzia Cuccu[3], Christian Fuchs[4], Kenji Watanabe[5], Takashi Taniguchi[5], Alexey Chernikov[3], Kerstin Volz[4], Sangam Chatterjee[2], and Andreas Knorr[1] — [1]ITP, Technische Universität Berlin, D-10623 — [2]LaMa, Justus-Liebig-University Giessen, D-35392 — [3]IAPP and ct.qmat, Technische Universität Dresden, D-01062 — [4]WZMW, Philipps-University Marburg, D-35032 — [5]NIMS, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan

In this joint theory-experiment collaboration, we study the Rabi splitting of excitons under simultaneous strong light-matter and Coulomb interaction on ultrafast timescales.

It turns out, that in a setting, where Coulomb and optical interaction are comparable (MQW), the Rabi splitting almost linearly follows the optical field amplitude similar to an ideal two-level system. On the other hand, in a setting with dominating Coulomb interaction ($MoSe_2$), the Rabi splitting depends sublinearly on the optical field strength and it significantly deviates from an ideal two-level system. Within the developed theoretical approach based on Heisenberg equations of motion and a correlation expansion of many-body interactions, we identify the origin of this sublinear trend due to six-particle exciton-to-biexciton transitions.

HL 40.12 Wed 18:30 H15

Inhomogeneous Broadening of Dark Rydberg Excitons in TMDC Monolayers Probed by Ultrafast Frequency-Resolved Autocorrelation Spectroscopy — •Katem Mitkong, Tom Jehle, Daniel C. Lünemann, Lukas Lackner, Juanmei Duan, Christian Schneider, and Christoph Lienau — Institute of Physics, Carl von Ossietzky University, Oldenburg, Germany

Monolayers of Transition Metal Dichalcogenides (TMDCs), as two-dimensional materials, exhibit unique optical properties influenced by their dielectric environment. The reduced dimensionality enhances the exciton binding energy, enabling the formation of Rydberg exciton series even at room temperature. In this study, broadband nonlinear Interferometric Frequency-Resolved Autocorrelation (IFRAC) spectroscopy with few-cycle time resolution is used to probe the optically dark 2p exciton state in WS2 monolayers. The result readily distinguishes coherent second harmonic generation (SHG) from incoherent two-photon photoluminescence emission (TPPLE) without requiring polarization control. We observe the 2p dark exciton state at 2.20 eV, with TPPLE linewidths that depend on excitation power. Comparison with Lindblad Master equation solutions shows significant inhomogeneous broadening of the 2p resonance, about three times greater than that of 1s excitons. This broadening, attributed to the extended spatial wavefunction of 2p excitons relative to 1s excitons, underscores their increased sensitivity to inhomogeneities such as local strain and dielectric fluctuations. This finding suggests potential applications in nanoscale sensing technologies.

HL 40.13 Wed 18:45 H15

Expanding the lithography toolbox - 2D devices and beyond — •Vasilis Theofylaktopoulos — Heidelberg Instruments Nano AG, Bändliweg 30, 8048 Zurich, Switzerland

Lithography is used in 2D devices to contact them with precisely placed electrodes, shape the building blocks or to control other properties such as doping or strain. Thermal scanning probe lithography is an up and coming method that can assist in all of the above.[1] In this talk the working principle of tSPL will be introduced and examples of its application will be given in the field of 2D electronics, photonics and metasurfaces.[2,3,4]

The NanoFrazor is a tSPL tool offering complimentary features to established lithography techniques such as photolithography, ebeam and focused ion beam. It uses a heated cantilever to write features with sizes bellow 15nm. At the same time grayscale patterning is possible with a resolution of 2nm. A reader is integrated at the tip allowing for parallel imaging to the patterning enabling markerless overlay. This simplifies the placement of features on 2D materials which are easily imaged under the resist. A laser can be used with the same resist stacks to create larger features >500nm such as contact pads. Finally, the process patterning the resist through sublimating it can yield devices with better electronics properties compared to ebeam.[5]

[1] S. T. Howell, A. Grushina, F. Holzner, and J. Brugger, Thermal scanning probe lithography - a review, Microsyst. Nanoeng., vol. 6, no. 1, p. 21, Apr. 2020, doi: 10.1038/s41378-019-0124-8.

[2] X. Liu et al., Thermomechanical Nanostraining of Two-Dimensional Materials, Nano Lett., vol. 20, no. 11, pp. 8250-8257, Nov. 2020, doi: 10.1021/acs.nanolett.0c03358.

[3] M. C. Giordano, G. Zambito, M. Gardella, and F. Buatier De Mongeot, Deterministic Thermal Sculpting of Large Scale 2D Semiconductor Nanocircuits, Adv. Mater. Interfaces, vol. 10, no. 5, p. 2201408, Feb. 2023, doi: 10.1002/admi.202201408.

[4] N. Marcucci, M. C. Giordano, G. Zambito, A. Troia, F. Buatier De Mongeot, and E. Descrovi, Spectral tuning of Bloch Surface Wave resonances by light-controlled optical anisotropy, Nanophotonics, vol. 12, no. 6, pp. 1091-1104, Mar. 2023, doi: 10.1515/nanoph-2022-0609.

[5] A. Conde-Rubio, X. Liu, G. Boero, and J. Brugger, Edge-Contact MoS2 Transistors Fabricated Using Thermal Scanning Probe Lithography, ACS Appl. Mater. Interfaces, vol. 14, no. 37, pp. 42328-42336, Sep. 2022, doi: 10.1021/acsami.2c10150.

HL 41: Spin Phenomena in Semiconductors

Time: Wednesday 15:45–16:30 Location: H17

HL 41.1 Wed 15:45 H17

The charge cycle of the silicon vacancy in diamond — •Joshua Claes, Bart Partoens, and Dirk Lamoen — University of Antwerp, Antwerp, Belgium

Color centers in wide bandgap semiconductors are point defects with strongly localized electrons, resembling atom-like systems that can be optically controlled. These defects hold great promise for advancing quantum technologies, including quantum sensing and quantum computing. Among them, the silicon vacancy (SiV) center in diamond stands out as a particularly promising candidate due to its narrow optical emission and long spin coherence time, lasting up to 1 second at cryogenic temperatures in its neutral state.

A key challenge for the practical use of such defects is the precise measurement of their spin state. Photoelectric detection of magnetic resonance (PDMR) is a promising technique that measures the spin state by inducing charge state transitions and capturing the released electron or hole. In this work, we employ density functional theory with the HSE06 hybrid functional to calculate the onset energies and optical cross-sections for charge state transitions of the SiV center in diamond, ranging from -2 to 0.

Using this data, we model the PDMR experiment to predict charge transitions as a function of the laser frequency applied, providing insights into the defect's behavior under experimental conditions.

HL 41.2 Wed 16:00 H17

Carrier spin coherence in inas/inalgaas quantum dots emitting in the telecom range — •Vitalie Nedelea — Technische Universität Dortmund, Dortmund, Germany

This study focuses on the carrier spin coherence in quantum dots(QDs), which are promising candidates for entanglement with an emitted photon as well as entanglement of two remote spins induced by measuring of two indistinguishable photons. The Samples, grown by molecular beam epitaxy, consist of 5.5nm InAs monolayers separated by InAlGaAs barriers. A Si δ-doped layer, at a distance of 15 nm from the QD layer, provides resident electrons. Differential transmission reveals a double exponential decay behaviour, with a short exciton(X) decay time of 0.5ns and the long indirect molecular X decay time of 2ns. The dependence of the Larmor frequencies on the transversal magnetic field (BV) gives us information about the carrier g-factor, |ge|=1.88 for the electron and |gh|=0.6 for the hole. The hole spin dephasing saturates at a higher value of T2*=1.4ns than the electron T2*=0.6ns, which could be explained by the weaker hyperfine coupling of the hole. The decay of the FR signal as a function of fm gives TS=0.3μs and extrapolating the power dependence to zero gives the spin relaxation time T1=0.5μs. The wide spread of g-factors and long spin relaxation times are promising candidates for the spin mode locking (SML) effect. In the ensemble of QDs, the sum of the multiple oscillating signals with Larmor frequencies corresponding to ωR contributes to the SML. Measured dependence of the SML on the BV reveal that the signal is related to the hole spins.

HL 41.3 Wed 16:15 H17

Optically induced spin electromotive force in ferromagnetic-semiconductor quantum well structure — •Olga Ken[1,2], Igor Rozhansky[2], Ina Kalitukha[1,2], Grigory Dimitriev[2], Mikhail Dorokhin[3], Boris Zvonkov[3], Dmitri Arteev[2], Nikita Averkiev[2], and Vladimir Korenev[2] — [1]TU Dortmund, Dortmund, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Lobachevsky State University of Nizhny Novgorod, Russia

We study hybrid structures which consist of ferromagnetic (FM) layer and a semiconductor quantum well (QW) and present here a systematic approach combining the optical and electrical detection of the spin-dependent electron transfer with nanoscale spatial resolution. Spin-dependent transfer is manifested in three spectacular effects: PL circular polarization under unpolarized excitation, dependence of the PL intensity from the QW on the circular polarization degree of the excitation, and spin-dependent photo-voltage across the junction. We show that in GaMnAs/GaAs/InGaAs heterostructure all the three parameters demonstrates similar non-linear magnetic field dependences with hysteresis loop saturating in ~100 mT [1]. This indicates the interaction of charge carriers in the QW with the FM, i.e. the FM proximity effect [2].

[1] I.V. Rozhansky et al. Nano Letters 23, 3994 (2023).
[2] V. L. Korenev et al. Nature Commun. 3, 959 (2012).

HL 42: Quantum Dots and Wires: Optics I

Time: Wednesday 16:45–18:30 Location: H17

Invited Talk HL 42.1 Wed 16:45 H17

Quantum key distribution with single photons from quantum dots — Joscha Hanel[1], •Jingzhong Yang[1], Jipeng Wang[1], Vincent Rehlinger[1], Zenghui Jiang[1], Frederik Benthin[1], Tom Fandrich[1], Jialiang Wang[1], Fabian Klingmann[2], Raphael Joos[3], Stephanie Bauer[3], Sascha Kolatschek[3], Ali Hreibi[4], Eddy. Patrick Rugeramigabo[1], Michael Jetter[3], Simone. Luca Portalupi[3], Michael Zopf[1,5], Peter Michler[3], Stefan Kueck[4], and Fei Ding[1,5] — [1]Leibniz Universität Hannover, Hannover, Germany — [2]Fraunhofer-Institut für Photonische Mikrosysteme, Dresden, Germany — [3]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [5]Laboratorium für Nano-und Quantenengineering, Hannover, Germany

Quantum key distribution (QKD) ensures secure communication against eavesdroppers. On-demand quantum light sources, such as semiconductor quantum dots (QDs), enhance QKD security and loss tolerance due to their deterministic single-photon emission with high brightness and low multiphoton rates. Here, we demonstrate high-speed modulation of telecom C-band single photons emitted from a QD embedded in a circular Bragg grating. Using a phase-modulator in a Sagnac-loop interferometer, a 16-bit pseudo-random sequence is encoded into polarisation states in real time at a 76 MHz clock rate, achieving an ultra-low quantum bit error rate of ~1%.

HL 42.2 Wed 17:15 H17

Development and deterministic fabrication of electrically controlled quantum dot molecule bullseye resonators — •Setthanat Wijitpatima[1], Normen Auler[2], Binamra Shrestha[2], Sven Rodt[1], Arne Ludwig[3], Dirk Reuter[2], and Stephan Reitzenstein[1] — [1]Institute of Solid-State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Department of Physics, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

Quantum information can be encoded in the polarization states of photons as flying qubits and decoded in the spin states of solid-state systems as stationary qubits, providing robust platforms for quantum information processing. Quantum dot molecules (QDMs) are particularly promising for this purpose, as their singlet-triplet qubits are immune to spin dephasing, enabling temporally stable spin-photon interfaces. Toward real-world applications, QDM devices with high photon extraction efficiency (PEE) are required, motivating the integration of QDMs into nanophotonic structures, such as circular Bragg gratings

(CBGs) which yield broadband enhancement of PEE and moderate Purcell enhancement. However, applying the CBG concept to QDMs has been challenging since precise electrical control is crucially needed to operate QDMs properly. In this work, we demonstrate the fabrication of QDM-CBG devices, providing a crucial step toward scalable and efficient quantum technologies.

HL 42.3 Wed 17:30 H17

Magnetic field dependence of the Auger recombination rate in a single quantum dot — •Nico Schwarz[1], Fabio Rimek[1], Hendrik Mannel[1], Marcel Zöllner[1], Britta Maib[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

In solid state physics, the quantum dot (QD) as a single photon emitter is an ideal system to study the Auger effect in a confined nanostructure. The Auger effect is an electron-electron scattering effect in which the energy of the electron-hole recombination is transferred to a third carrier, leading to a non- radiative recombination of, e.g., the trion [1]. This Auger recombination should be suppressed in high-photon-yield, low-dephasing single-photon emitters. We used two-color, time resolved resonance fluorescence spectroscopy with a high spectral resolution on a single quantum dot to differentiate between the differ- ent recombination paths: Auger, spin-flip and spin-flip Raman recombination [2]. We observe an unexpected behaviour of the Auger recombination rate, which shows a decrease from B = 0 to 2 T, followed by an increase to 4 T , before decreasing again by a factor of approx. three up to 8 T. These new findings may be the starting point for further theoretical and experimental studies to unterstand or even supress this scattering effect, in which the environment seems to play an important role. [1] P. Lochner et al., Nano Lett. **20**, 1631-1636 (2020). [2] H. Mannel et al., JAP **134**, 154304 (2023).

HL 42.4 Wed 17:45 H17

Studying the optical properties of AgInS2-based quanutm dots — •Yizhuo Xi, Julian Mann, Jochen Feldmann, and Sushant Ghimire — Chair for photonics and optoelectronics, Nanoinstitute Munich and department of physics, Ludwig-Maximilians-University, Königstr.10, 80539 Munich, Germany

I-III-VI quantum dots have attracted considerable interest for their non-toxic nature, tunable bandgap, and excellent stability. However, these quantum dots contain intrinsic sub-gap defects, which can act as donor-acceptor pairs. In this work, we synthesize AgInS2 quantum dots showing a dual emission spectrum. A narrow but weak free-exciton emission is observed near the band edge, while a broad and intense emission, associated with donor-acceptor-type defects, appears in the lower energy region. After coating the core particles with a gallium sulfide shell, the free-exciton luminescence is strongly improved, and the recombination at donor-acceptor pairs is suppressed. This demonstrates the successful elimination of defects in AgInS2/GaSx core/shell quantum dots, which is further evidenced in the absorption spectrum by the removal of a defect-related Urbach tail. In essence, we find that the donor-acceptor pair defects in these AgInS2 quantum dots are mainly located on the surface, and the excitonic character emerges upon their elimination through the growth of a gallium sulfide shell.

HL 42.5 Wed 18:00 H17

Deoxidization induced InAs(P) single photon emitter formation on InP substrate — •Yiteng Zhang[1], Xin Cao[1], Doaa Abdelbarey[1], Zenghui Jiang[1], Markus Etzkorn[2], Chenxi Ma[1], Tom Fandrich[1], Arijit Chakraborty[1], Tom Rakow[1], Eddy Rugeramigabo[1], Michael Zopf[1,3], and Fei Ding[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167, Hannover, Germany — [2]Technische Universität Braunschweig,LENA, Institut für Angewandte Physik, Universitätsplatz 2, 38106 Braunschweig — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167, Hannover, Germany

Efficient quantum light sources at telecom O-band and C-band are essential for long-haul quantum communication to minimize photon dispersion and loss. While semiconductor quantum dots (QDs) grown by Stranski-Krastanov and droplet epitaxy methods show promise, their reproducibility is hindered by complex growth parameters. Here, we present a straightforward method to fabricate self-assembled InAs(P) QDs emitting single photons at telecom O-band using molecular beam epitaxy. By deoxidizing and annealing InP(001) substrates in an arsenic atmosphere, QDs form naturally without additional metal deposition. Statistical analysis reveals size distribution and density comparable to QDs from conventional methods. Cryogenic photoluminescence confirms single-photon emission. This approach offers a reproducible and efficient pathway to telecom-wavelength single-photon sources, advancing quantum information technologies.

HL 42.6 Wed 18:15 H17

Excitonic structure of G center computed by unfolded tight-binding model — •Jakub Valdhans[1] and Petr Klenovský[1,2] — [1]Masaryk University, Brno, Czech Republic — [2]Czech Metrology Institute, Brno, Czech Republic

We have studied the carbon G center in bulk silicon and germanium using the empirical tight-binding (ETB) model for calculating unfolded band structures with configuration interaction (CI) correction for an exciton. The G center in B configuration (emissive) being a candidate for a telecom single photon source has two substitutional carbons and one interstitial atom embedded in the bulk for 6 possible configurations. Using advantage of low computation effort of ETB, it is possible to calculate and analyze behavior of electronic transitions with respect to a variation of bond distance between substitutional carbons and interstitial atom, and with using band offset as external tuning parameter.

HL 43: Twisted Materials / Systems (joint session TT/HL)

Time: Wednesday 17:00–18:30 Location: H31

HL 43.1 Wed 17:00 H31

Formation, persistence and ordering of local moments in magic angle twisted bilayer graphene — •Lorenzo Crippa[1,2], Gautam Rai[1], Dumitru Călugăru[3,13], Haoyu Hu[4], Luca de' Medici[5], Antoine Georges[6,7,8,9], Bogdan Andrei Bernevig[3,4,10], Roser Valentí[11], Giorgio Sangiovanni[2], and Tim Wehling[1,12] — [1]University of Hamburg — [2]University of Würzburg — [3]Princeton University — [4]DIPC, Donostia-San Sebastian — [5]ESPCI, Paris — [6]Collège de France, Paris — [7]Flatiron Institute, New York — [8]École Polytechnique, Palaiseau Cedex — [9]Université de Genève — [10]IKERBASQUE, Bilbao — [11]Goethe University Frankfurt — [12]Hamburg CUI — [13]University of Oxford

The physics of magic angle twisted bilayer graphene (MATBLG) is remarkably diverse across a wide range of dopings and temperatures.

By means of a Dynamical Mean-Field Theory (DMFT) approach, we study the effect of electronic correlations in MATBLG, with particular focus on the physics of local spin and valley isospin moments. We analyze their magnitude and screening across a broad temperature range, discuss the limits of very low and infinite temperature, and obtain two different scales for their formation (around 100 K) and ordering (around 10 K).

We discuss their implications in terms of transport properties of the system (e.g. resistivity) and of spectral features (resonance peaks) and contextualize our findings with recent experimental results.

HL 43.2 Wed 17:15 H31

Nematic versus Kekulé phases in twisted bilayer graphene under hydrostatic pressure — Miguel Sánchez Sánchez[1], Israel Díaz[1], José González[2], and •Tobias Stauber[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC — [2]Instituto de Ciencia de Materiales, CSIC

We address the precise determination of the phase diagram of magic angle twisted bilayer graphene under hydrostatic pressure within a self-consistent Hartree-Fock method in real space, including all the remote bands of the system. We further present a novel algorithm that maps the full real-space density matrix to a 4x4 density matrix based on a SU(4) symmetry of sublattice and valley degrees of freedom. We find a quantum critical point between a nematic and a Kekulé phase, and show also that our microscopic approach displays a strong particle-

hole asymmetry in the weak coupling regime. We arrive then at the prediction that the superconductivity should be Ising-like in the hole-doped nematic regime, with spin-valley locking, and spin-triplet in the electron-doped regime [1].

[1] M. Sánchez Sánchez, I. Díaz, J. González, T. Stauber, Phys. Rev. Lett. (in press), arXiv:2403.03140.

HL 43.3 Wed 17:30 H31

Quantum diffusion in sheared bilayer graphene — •Taher Rhouma[1], Florie Mesple[2], Vincent Renard[3], and Guy Trambly de Laissardière[1] — [1]LPTM, CY Cergy Paris Univ., CNRS, Cergy-Pontoise, France. — [2]Dept. Physics, Univ. of Washington, USA — [3]CEA, Univ. Grenoble Alpes, IRIG, PHELIQS, Grenoble, France

The identification of correlated insulators and superconductivity in magic-angle twisted bilayer graphene (MATBG) has sparked significant interest in its electronic properties [1]. When examining the MATBG moiré patterns along the line with alternating regions of AA, AB, and BA, we observe striking similarities to those found in a 1D moiré of a sheared bilayer graphene, where one layer is laterally displaced. That may lead to a localization of the electronic states [2]. In this study, we investigate numerically the electronic and quantum transport properties in sheared bilayer graphene, focusing on how the degree of shear influences these characteristics.

[1] Y. Cao, et al., Nature **556**, 43 (2018); Nature **556**, 80 (2018).
[2] J. Gonzalez, Phys. Rev. B **94**, 165401 (2016).

HL 43.4 Wed 17:45 H31

Ab-initio fRG study on tWSe$_2$ — •Hannes Braun — Max Planck Institut für Festkörperforschung — Technische Universität München

The recent experimental reports on superconductivity in twisted WSe_2 have served to justify the already considerable interest in twisted TMD systems. From a theoretical standpoint, there have been numerous attempts to describe these systems. To study the phase diagram and analyse the governing physics, we employ the functional renormalisation group method. This approach allows us to gain an unbiased understanding of the interplay between fluctuations leading to symmetry-broken phases. To develop a model capable of describing the material, we integrate *ab-initio* results as initial conditions. In this talk, we present method developments for a more efficient momentum integration and results on the interplay between magnet and pairing instabilities.

HL 43.5 Wed 18:00 H31

Mott transitions and doping asymmetry in twisted bilayer WSe$_2$ — •Siheon Ryee[1], Lennart Klebl[2,1], Valentin Crépel[3], Ammon Fischer[4], Lede Xian[5,6], Angel Rubio[6,3], Dante Kennes[4,6], Andrew Millis[3,7], Antoine Georges[8,3], Roser Valentí[9], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany — [3]Flatiron Institute, New York, USA — [4]RWTH Aachen University, Aachen, Germany — [5]Tsientang Institute for Advanced Study, Zhejiang, China — [6]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [7]Columbia University, New York, USA — [8]Collège de France, Paris, France — [9]Goethe Universität Frankfurt, Frankfurt am Main, Germany

The recent discovery of superconductivity in twisted bilayer WSe_2 ($tWSe_2$) at two distinct twist angles (3.65 deg and 5 deg) along with previous reports of metal-insulator transitions, spin density wave states, and fractional Chern insulators raises deep questions in correlated electron physics. We present results of a dynamical mean-field theory-based investigation of a model that faithfully captures the band structure and topology of twisted transition metal dichalcogenides as functions of twist angle and displacement field. We find good agreement with several key aspects of the experimental data. Focusing further on the twist angle of 3.65 deg, we discuss the nature of the electric-field-induced metal-insulator transition, the experimentally observed coherence temperature, and the origin of the observed doping asymmetry in resistivity.

HL 43.6 Wed 18:15 H31

Twisted bilayer MoS$_2$ under electric fields: A system with tunable symmetry — •Aitor Garcia-Ruiz[1,2] and Ming-Hao Liu[1] — [1]National Cheng Kung University, Tainan, Taiwan — [2]National Graphene Institute, University of Manchester, Manchester, United Kingdom

Gate voltages take full advantage of two-dimensional systems, making it possible to explore novel states of matter by controlling their electron concentration or applying perpendicular electric fields. Here, we study the electronic properties of small-angle twisted bilayer MoS_2 under a strong electric field. We show that the transport across one of its constituent layers can be effectively regarded as a two-dimensional electron gas under a nanoscale potential. We find that the band structure of such system reconstructs following two fundamentally different symmetries depending on the orientation of the external electric field, namely, hexagonal or honeycomb. By studying this system under magnetic fields, we demonstrate that this duality not only translates into two different transport responses, but also results in having two different Hofstadter's spectra. Our work opens up a new route for the creation of controllable artificial superlattices in van der Waals heterostructures.

HL 44: Focus Session: Quantum Technologies in Deployed Systems I

Recent advancements in quantum cryptography, quantum computing, and quantum sensing are driving researchers to develop a universal quantum network*known as the quantum internet, which will enable secure connections among quantum computers, as well as to networks of quantum sensors, through quantum cryptography. Building a functional quantum internet is one of the most ambitious goals in quantum technology for the coming decades.

The focus sessoin aims to provide a comprehensive overview of the corresponding platforms and advances in quantum technologies, and is organized by Simone L. Portalupi (U. Stuttgart), Michal Vyvlecka (U. Stuttgart) and Michael Zopf (U. Hannover).

Time: Wednesday 18:00–18:45 Location: H13

HL 44.1 Wed 18:00 H13

Advancing Quantum Communication with Deterministic Quantum Light Sources from Laboratory- to Field-Experiments — •Mareike Lach, Koray Kaymazlar, Pratim Saha, Martin von Helversen, and Tobias Heindel — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

The advances in the field of non-classical light generation using solid-state quantum light sources fostered the exploration of applications in quantum communication and networking. This interdisciplinary field thereby increasingly evolves from laboratory-scale to field-experiments [1]. In this contribution we address the design, set-up and characterization of stand-alone compact modules for field-deployable quantum communication systems. In this context key components of the transmitter- and receiver-stations for quantum key distribution protocols are discussed, including mobile quntum light sources, fast qubit-state encoders, and qubit-state analyzers. Advancing the field-deployment of quantum technologies will foster both the progress in explorativ research projects as well as the transfer to their commercialization.

[1] D.A. Vajner et al., Advanced Quantum Technologies, doi:10.1002/qute.202100116 (2022)

HL 44.2 Wed 18:15 H13

Automated in situ optimization and disorder mitigation in a quantum device — •Jacob Benestad[1], Torbjørn Rasmussen[2,3], Bertram Brovang[2], Oswin Krause[4], Saeed Fallahi[5,6], Ge-

offrey C. Gardner[6], Michael J. Manfra[5,6,7,8], Charles M. Marcus[2], Jeroen Danon[1], Ferdinand Kuemmeth[2], Anasua Chatterjee[2,3], and Evert van Nieuwenburg[9] — [1]Department of Physics, Norwegian University of Science and Technology — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — [3]QuTech and Kavli Institute of Nanoscience, Delft University of Technology — [4]Department of Computer Science, University of Copenhagen — [5]Department of Physics and Astronomy, Purdue University — [6]Birck Nanotechnology Center, Purdue University — [7]Elmore Family School of Electrical and Computer Engineering, Purdue University — [8]School of Materials Engineering, Purdue University — [9]Lorentz Institute and Leiden Institute of Advanced Computer Science

We investigate automated in situ optimisation of a quantum point contact (QPC) device with 9 adjustable electrostatic gates atop the split-gate constriction, using the Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) with a metric for how "step-like" the conductance is when the channel is constricted. The optimization algorithm is first tested on tight-binding simulations to show how it could adapt to a disorder potential, followed by implementing it in an experiment to show a marked improvement in the quantization of device conductance.

HL 44.3 Wed 18:30 H13

Fast and high-fidelity composite gates in superconducting qubits: Beating the Fourier leakage limit — •Hristo Tonchev[1], Boyan Torosov[2], and Nikolay Vitanov[1] — [1]Center for Quantum Technologies, Department of Physics, Sofia University, James Bourchier 5 blvd., 1164 Sofia, Bulgaria — [2]Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko chaussée, 1784 Sofia, Bulgaria

We present a method for quantum control in superconducting transmon qubits, which overcomes the Fourier limit for the gate duration imposed by leakage to upper states. The technique utilizes composite pulses, which allow for the correction of various types of errors that naturally arise in a system. We use our approach to produce complete and partial population transfers between the qubit states, as well as two basic single-qubit quantum gates. Our simulations show a substantial reduction of the typical errors and gate durations. Three different independent verifications are made to justify these claims.

HL 45: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:00 Location: H13

HL 45.1 Thu 9:30 H13

Optical Simulations of Nanophotonic Back Contacts for Light Management in Ultrathin CIGSe Solar Cells — •Daniel Jiménez Tejero[1], Merve Demir[1], Bodo Fuhrmann[2], Roland Scheer[1], Ralf Wehrspohn[1], and Alexander Sprafke[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle (Saale) — [2]MLU, Interdisziplinäres Zentrum für Materialwissenschaften, Nanotechnikum Weinberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

The development of ultrathin-film Cu(In,Ga)Se_2 (CIGSe) solar cells aims to reduce material usage and expand applications such as bifacial or tandem solar cells. However, CIGSe absorber layers with thicknesses below 1 μm exhibit diminished light absorption, particularly for wavelengths near the bandgap, leading to decreased power conversion efficiency. This can be counteracted by utilising functional back contacts that effectively increase the optical path length within the absorber layer through scattering, reflection, and nanophotonic mechanisms.

This work employs nano-optical simulations to investigate the potential of SiO_2 nanostructures on a flat gold back contact for enhancing the performance of CIGSe solar cells. By solving the Maxwell equations using the finite element method, the quantum efficiency and photocurrent under ideal charge carrier collection conditions are computed, enabling a comparison of various nanostructure geometries viable for fabrication. We find photocurrents higher than those of conventional CIGSe solar cells with an absorber thickness of 4 μm, indicating the potential of our light management approach.

HL 45.2 Thu 9:45 H13

Stabilizing Perovskite Solar Cells by Organic Salts Under One Full Sun and Maximum Power Point Tracking — •Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Bashudev Bhandari[2,3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany

The use of organic halide salts to passivate metal halide perovskite (MHP) surfaces have been studied extensively. Passivating the surface defects of the MHP is of critical importance for realizing high-efficiency and stability of perovskite solar cells (PSCs). Here we discuss the success of a multifunctional organic salt used as passivation material for grain boundary defects and as molecular sealing layer in terms of stabilization. To assess the stability of PSCs, maximum power point tracking is seemingly the most realistic condition for the ageing test. Here, PSCs made from the four cation RbCsMAFA based perovskite absorber layer were aged under full light with maximum power point tracking and in addition they were tested periodically by IV-characterization, in order to yield all photovoltaic parameters for improved understanding of the ageing process.

HL 45.3 Thu 10:00 H13

Hyperuniform discordered structures for Light Management in Ultrathin CIGSe Solar Cells — •Katharina Trockel[1], Merve Demir[1], Frank Syrowatka[2], Ralf Wehrspohn[1], Roland Scheer[1], and Alexander Sprafke[1,2] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Interdisciplinary Center of Materials Science, 06120 Halle, Germany

Ultrathinfilm Cu(In,Ga)Se2 (CIGSe) solar cells are highly attractive due to their reduced material consumption and low manufacturing costs. While conventional CIGSe solar cells can achieve efficiencies of up to 21 %, increasing the efficiency of ultrathin solar cells remains a key research objective to enhance their competitiveness. A promising approach involves extending the optical path length in the absorber layer by integrating textured structures at the back or front contact of the solar cell. Most studies focus on periodic textures.

In this work, we investigate hyperuniform disordered (HuD) structures for light management in ultrathin CIGSe solar cells. The HuD structures are fabricated using polymethyl methacrylate (PMMA) particles deposited onto the back contact of the solar cells. These particles are covered with an indium tin oxide (ITO) layer and subsequently removed via a calcination process. The resulting ITO layer functions as a textured back contact, improving both light scattering and electrical performance.

First experimental results on the implementation of CIGSe solar cells with integrated HuD structures will be presented.

HL 45.4 Thu 10:15 H13

A Theoretical study of charge transport properties in perovskite analogues for high performance solar cells. — •Prerna Prerna[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Perovskite materials have emerged as promising candidates in solar cell technology, offering exceptional efficiency and affordability. Their remarkable performance, surpassing that of conventional inorganic materials, has placed them at the forefront of next-generation solar cell research, attracting significant attention from both academic and industry.

To harness their potential, we are investigating their charge transport properties using first-principles calculations (DFT) within the band transport regime. Our focus includes the calculation of carrier mobility, scattering rates and relaxation time through a detailed analysis of effective mass, deformation potential, and elastic properties. Our studies also incorporate the effects of structural deformations, aiming to align theoretical predictions with experimental results, providing deeper insights into the transport mechanisms in perovskites.

Furthermore, we are exploring the anisotropic nature of perovskites to understand directional dependencies in their electronic and mechanical properties. This anisotropy analysis is crucial for optimizing their performance and tailoring their application in advanced solar technologies. Together, these studies offer a comprehensive approach to enhancing the functionality of perovskites for cutting-edge solar energy solutions.

HL 45.5 Thu 10:30 H13

THz-Driven Phonon Fingerprints of Hidden Symmetry Breaking in 2D Layered Hybrid Perovskites — •Joanna M. Urban[1], Michael S. Spencer[1], Maximilian Frenzel[1], Gaëlle Trippé- Allard[2], Marie Cherasse[1,3], Charlotte Berrezueta Palacios[4], Olga Minakova[1], Luca Perfetti[3], Stephanie Reich[4], Martin Wolf[1], Emmanuelle Deleporte[2], and Sebastian F. Maehrlein[1,5,6] — [1]FHI Berlin — [2]LuMIn, Université Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS — [3]LSI, CEA/DRF/IRAMIS, CNRS, École Polytechnique, Institut Polytechnique de Paris — [4]FU Berlin — [5]HZDR — [6]TU Dresden

Metal halide perovskites (MHPs) are emerging as promising candidates for spintronic applications. In MHPs which lack inversion symmetry, strong spin-orbit coupling induces the Rashba-Dresselhaus effect, allowing spin current control. Here we use intense THz fields to coherently drive lattice dynamics in Ruddlesden-Popper 2D layered perovskites. We identify simultaneous IR and Raman activity of specific inorganic cage modes, suggesting the presence of inversion symmetry breaking despite the globally centrosymmetric crystal structure. By exploring the driving pathways of coherent phonons bearing the signatures of broken inversion symmetry, we lay the groundwork for simultaneous ultrafast control of optoelectronic and spintronic properties in 2D MHPs.

HL 45.6 Thu 10:45 H13

Analysis of real-space transport channels in halide perovskites — •Frederik Vonhoff[1], Maximilian J. Schilcher[1], David R. Reichman[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA

The charge carrier transport is a crucial factor for the performance of halide perovskites as solar energy conversion material. However, standard semiconductor transport theories fail to model the transport properties of halide perovskites because of their unusual transport behavior triggered by the anharmonic nuclear dynamics and its dynamic disorder [1]. For an accurate prediction of electron and hole mobilities of $MAPbI_3$ and $MAPbBr_3$, we capture the anharmonicity with molecular dynamics trajectories as a backbone for a time-dependent real-space hopping model [2,3] parametrized with hybrid density functional theory. With our transport model, we trace back the transport behavior of $MAPbI_3$ and $MAPbBr_3$ to their band structures via the projected density of states and the dynamics in the orbital occupation configurations. The real-space nature of our model allows us to determine the microscopic transport mechanisms which are driven by three transport channels.

[1] M. J. Schilcher et al, ACS Energy Lett. 6, 2162 (2021)
[2] M. Z. Mayers et al, Nano Lett. 18, 8041 (2018)
[3] M. J. Schilcher et al, Phys. Rev. Mater. 7, L081601 (2023)

15 min. break

HL 45.7 Thu 11:15 H13

Unravelling how solvated PbI_2 Crystallites precede the Crystallization of Lead Halide Perovskites by UV/VIS In-Situ measurements — •Maximilian Spies[1], Simon Biberger[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth, Germany — [2]Dynamics and Structure Formation, University of Bayreuth, Bayreuth, Germany

The fabrication of reproducible, high-quality lead iodide perovskite films via solution-based methods requires a comprehensive understanding of crystallization dynamics. The formation of perovskite films is primarily dictated by the composition of the precursor solution and its processing conditions. In this study, we present an in-situ absorption study, i.e. during spin-coating, of the critical pre-nucleation stage to unravel the formation mechanisms of lead iodide perovskite films. We tracked the evolution of iodoplumbate complexes within the precursor solution and identified a distinctive absorption feature at 3.15 eV, emerging prior to film formation. We attribute this feature to the development of a crystalline PbI_2-DMF solvated (PDS) phase. In particular, we propose that PDS crystallites serve as precursors to the crystalline perovskite phase, acting as nucleation sites within the precursor solution. Notably, the amount of this PDS phase correlates closely with the concentration of the solution layer during spin coating, suggesting that increasing concentration promotes PDS formation. These findings provide valuable insights into the early stages of perovskite crystallization.

HL 45.8 Thu 11:30 H13

Effect of a 2D/3D Heterostructure on Contact Formation of the Double Perovskite $Cs_2AgBiBr_6$ with Hole Transport Layers Revealed by In-Situ KPFM Growth Studies — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of a 2D perovskite interlayer caused by surface modification with organic amines between the absorber and contact layers is widely known to significantly improve the performance of perovskite solar cells. This has already been approved as well for the lead-free double perovskite absorber $Cs_2AgBiBr_6$. To better understand the interaction of the contact layer with the 2D/3D heterostructure, in this work, film growth of Copper Phthalocyanine (CuPc), used as a model hole conductor, onto $Cs_2AgBiBr_6$ modified by different 2D phases was investigated and compared to bare $Cs_2AgBiBr_6$. Employing solar cell geometry, the morphology and work function were inspected intermittently to the evaporation of CuPc by Kelvin Probe Force Microscopy at different average film thickness. The energy alignment was revealed to be more confined on the 2D/3D heterostructures and the growth of CuPc was improved: a more homogenous growth led to formation of closed films even at early stages of deposition. These changes in growth and energy alignment are accompanied by preferential formation of different crystal phases in the CuPc.

HL 45.9 Thu 11:45 H13

The influence of oxygen and water on $MAPbI_3$ absorber materials measured with in-situ TRPL and PES — •P. Stötzner[1], M. Müller[1], T. Schulz[1], P. Pistor[2], R. Scheer[1], and S. Förster[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Universidad Pablo de Olavide Sevilla, Spain

Methylammonium lead halide perovskites ($MAPbI_3$) are promising thin-film solar cell absorber materials, but their response to environmental conditions like moisture and oxygen is not well understood. Here, we present a combined photoelectron spectroscopy (PES) and in-situ time-resolved photoluminescence (TRPL) study conducted in one ultrahigh vacuum system, which allows for studying changes in the chemical composition, the electronic structure and charge carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.
For $MAPbI_3$, we observe a significant reduction of the charge carrier lifetime compared to ex-situ TRPL measurements. To bridge between the different measurement environments, we conducted additional TRPL measurements in a closed cell having the as-grown sample in nitrogen atmosphere, which is pumped to high vacuum. These results show a decreased lifetime in vacuum but an increased lifetime linked to air contact. Consequently, we exposed $MAPbI_3$ samples to water vapor to mimic air contact, resulting in increased lifetime but also in a decomposition of $MAPbI_3$. Pure oxygen exposure did not affect the lifetime. Surprisingly, the simultaneous exposure to both gases did not show the detrimental effect of water.

HL 45.10 Thu 12:00 H13

On the Nature of Light Induced Defects in MAPI Thin Films: Long Pulses in TrPL — •Maxim Simmonds and Eva Unger — Kekuléstraße 5, 12489 Berlin, Germany

Metal-halide perovskite (MHP) semiconductors are highly relevant candidates for the fabrication of next generation solar cells but suffer from instability under continuous irradiation. This has been shown with a non-constant steady state PL during illumination. In order to better understand the evolution of recombination mechanisms at play, we usetime resolved photoluminescence (trPL) and differential lifetime plots.

Therefore, in this presentation, we will focus on methylammonium-lead-iodide (MAPI) thin films and the (ir)reversible introduction of traps triggered by quasi-continuous illumination. For this, we develop

a method that uses long pulses of light in combination with trPL counting schemes, calling it long pulsed trPL (LP-trPL). From the method, we observe the inclusion of long lived and non-deep trapping sites due to continuous illumination. The data also suggests a highly asymmetric mechanism of trap formation, where trap annihilation is much slower than observed formation. We conclude that previously described mechanisms of iodine outgassing is compatible with the observed shallow nature of traps introduced as well as the asymmetric process of formation/annihilation.

HL 45.11 Thu 12:15 H13

Phase evolution of sequential evaporated (FA/Cs)SnI_3 halide perovskite thin films via in situ X-ray diffraction — •Pu-Chou Lin[1], Josha Damm[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Photovoltaics Group, Martin-Luther-University, 06120 Halle, Germany — [2]Departamento de Sistemas Físicas, Universidad Pablo de Olavide, 41013 Sevilla, Spain

Tin-based halide perovskites, particularly $FASnI_3$ and $CsSnI_3$, offer promising potential for photovoltaic applications. This study employs in situ X-ray diffraction to investigate these materials' real-time growth mechanisms and thermal stability during sequential vapor deposition and annealing. Our results demonstrate that the deposition sequence significantly impacts the resulting perovskite film quality. For $FASnI_3$, the SnI_2-FAI stack yields superior, cavity-free films compared to the FAI-SnI_2 stack. This suggests that FAI is the primary diffusing species, with $FASnI_3$ forming at interfaces and completing its formation around 160°C. In contrast, the $CsSnI_3$ system exhibits more complex behavior. The SnI_2-CsI sequence leads to the formation of the intermediate phase Cs_2SnI_6, while the CsI-SnI_2 sequence directly forms $CsSnI_3$ with minimal defect formation. This suggests that SnI_2 is the dominant diffusing species in the Cs-based system. $FASnI_3$ and $CsSnI_3$ undergo thermal degradation at 200°C and 240°C, respectively, through co-desorption of their constituent elements. These findings provide valuable insights into tin-based perovskites' growth mechanisms and thermal stability, which can guide future efforts to improve their performance and long-term stability.

HL 45.12 Thu 12:30 H13

Determining the key parameters of 3C-SiC photoelectrodes for water splitting application — •Marius Wasem[1,2], Sebastian Benz[1,3], Philip Klement[1,2], Joachim Sann[1,3], Jürgen Janek[1,3], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

We investigated the photoelectrochemical properties of n- and p-doped 3C-SiC thin films on n- or p-doped Si substrates, respectively, in a phosphate buffer solution. Key parameters such as the flat band potential and open-circuit potential were determined using various electrochemical methods. The combination of ultraviolet photoelectron spectroscopy and low energy inverse photoelectron spectroscopy measurements yields the estimation of the positions of the Fermi level, as well as the positions of the valence and conduction bands of the differently doped 3C-SiC thin films. Impedance spectroscopy characterized the interfacial processes in more detail. The flat band potential was derived from the space-charge layer capacitance using Mott-Schottky analysis. The determination of these key parameters enabled the construction of an energy level diagram, which explains the electrochemical behavior of n- and p-type 3C-SiC thin films under both dark conditions and illumination.

HL 45.13 Thu 12:45 H13

Circular Dichroism Engineering via Bismuth Doping and Cation Substitution in 2D Lead-Halide Perovskites — •Jan-Heinrich Littmann[1], Keito Mizukami[1,2], Henrik Spielvogel[1], Philip Klement[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Hybrid lead halide perovskites have garnered significant attention for their remarkable semiconductor properties. Their building blocks allows for tuneable features such as the crystal structure and the electronic bandgap. Introducing chiral cations into these materials endows them with chiroptical properties, such as circularly polarized luminescence (CPL) and spin-polarized charge transport, promising applications in optoelectronics and spintronics. However, the mechanism of chirality transfer remains poorly understood due to complex structure-property relationships. This study delves into the impact of heterovalent Bi^{3+} doping on the genuine circular dichroism (CD) of 2D lead iodide perovskites incorporating methylbenzylamine (MBA) and (pyridyl)ethylamine (PyEA) cations. Bi^{3+} doping, while preserving the band gap, significantly influences the genuine CD, suggesting a doping-dependent chirality transfer mechanism. Our findings provide valuable insights into the structure-property relationships in chiral perovskites and pave the way for the rational design of advanced chiroptical materials.

HL 46: Optical Properties

Time: Thursday 9:30–13:00 Location: H15

Invited Talk HL 46.1 Thu 9:30 H15

Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, and Manfred Bayer — Experimentelle Physik 2a, TU Dortmund University, Dortmund, Germany

We demonstrate self-sustained auto-oscillations in a dissipative electron-nuclear spin system (ENSS) in semiconductors, where spontaneous breaking of translational symmetry in time produces robust limit-cycle dynamics across a broad range of parameters, including laser power, temperature, and magnetic field. These periodic oscillations exhibit coherence times extending to hours, reflecting ideal "time atom" ordering within the auto-oscillatory system.

Additionally, we uncover synchronization within excited subsystems without additional modulation, identifying its microscopic origins. Under periodic driving, modulation of parameters such as excitation power and pump polarization yields parametric resonances, signaling a transition to discrete auto-oscillatory behavior. Key phenomena include frequency entrainment, Arnold tongues, bifurcation jets, and a devil's staircase, showcasing the ENSS's versatility in exploring nonlinear dynamics, with broad implications for both fundamental physics and semiconductor applications.

HL 46.2 Thu 10:00 H15

Material selective Nonlinear Optics on Transition-metal Dichalcogenide - ZnO Nanowire Hybrid Structures — •Maximilian Tomoscheit, Benedikt Mathes, Edwin Eobalt, Alexander Zaunick, Carsten Ronning, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena

The nonlinear optical (NLO) properties of any material are described by the complex tensor $\boldsymbol{\chi}^{(n)}$, where, for each element of the tensor, the imaginary part mainly appears close to optical resonances. A direct measurement of the complex NLO suscebility is challenging because any NLO measurement is proportional to $|\boldsymbol{\chi}^{(n)}|^2$. A second harmonic generation (SHG) interference measurement from two different materials with $\boldsymbol{\chi}_\nu^{(2)}$ ($\nu = 1, 2$), is also proportional to $\left|\boldsymbol{\chi}_1^{(2)}\right|\left|\boldsymbol{\chi}_2^{(2)}\right|\cos\theta$, where θ is the phasemismatch. For a hybrid system with non overlapping resonances, if the SH photon energy is off-resonant for one material and resonant for the other, the interference term directly probes the complex NLO suscebility of the resonant material. In this work, we study SH interference in a transition-metal dichalcogenide (TMD) ZnO-nanowire (NW) hybrid structure, and we characterize the complex NLO suscebility of the TMD close to the A-exciton resonance. To be able to measure such interference, the ZnO NW needs to be placed along the armchair direction of the TMD, in our case WSe_2. Preliminary measurements and the results of SH polarization and wavelength dependent measurements will be be presented in this talk.

HL 46.3 Thu 10:15 H15

Nonempirical hybrid functional based on metaGGA — •Stefan Riemelmoser[1], Xun Xu[1,2], and Alfredo Pasquarello[1] — [1]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne,

Switzerland — [2]Beijing Computational Science Research Center, Beijing, China

Semi-local density functionals such as PBE typically underestimate experimental band gaps by 50%. Hybrid functionals address this "band gap problem" by admixing a fraction of exact exchange to semi-local exchange. The optimal mixing parameter depends on the specific material and can be identified as the inverse dielectric constant. Recently, we have show that dielectric constants obtained using the r^{2}SCAN metaGGA functional are significantly more accurate than dielectric constants obtained using PBE. This can be understood through the improved treatment of electronic self-interaction within the metaGGA framework.

In this talk, we will show that a dielectric-dependent hybrid functional based on r^{2}SCAN can outperform the standard PBE based hybrid in terms of band gaps. Particularly impressive improvements are obtained for narrow gap semiconductors such as Ge and InAs, where PBE wrongly predicts a metallic phase, but r^{2}SCAN can open a gap. The hybrid functional based on r^{2}SCAN also yields accurate effective masses and ionization potentials. Finally, we showcase that our new hybrid functional is an excellent choice for semiconductor applications such as defect calculations.

HL 46.4 Thu 10:30 H15

Room-temperature polariton condensate in a two-dimensional hybrid perovskite — •M. Struve[1], C. Bennenhei[1], H. P. Adl[1], K. W. Song[2], H. Shan[1], N. Mathukhno[1], J. Drawner[1], F. Eilenberg[3], N. P. Jasti[4], D. Cahen[4], O. Kyriienko[2], C. Schneider[1], and M. Esmann[1] — [1]Institut for Physics, Carl von Ossietzky Universität Oldenburg — [2]University Exeter, United Kingdom — [3]Frauenhofer IOF, Jena — [4]Weizmann Instutute of Science, Israel

Chemically synthesized 2D halide perovskites form naturally grown quantum well stacks. Their large binding energy, tunable emission spectra and high oscillator strength makes them promising platforms for room temperature polaritonics but bosonic condensation and polariton lasing at ambient conditions are yet to be shown. In this work we demonstrate cavity exciton-polariton condensation of 2D Ruddelson-Popper iodine perovskites $(BA)_2(MA)_2Pb_3I_{10}$ crystal at room temperature [1]. A polariton condensation threshold of $P_{th}\approx$6.8 fJ with a strong non-linear response is observed. The emergence of spontaneous spatial coherence across the condensate with interferometric measurements is confirmed with a first-order autocorrelation reaching $g^{(1)}\approx$0.6. With our results we lay the foundation for a new class of 2D halide perovskite based room-temperature polariton lasers that offer great potential for hetero-integration with other van-der-Waals materials and combination with photonic crystals. [1] M.Struve et al., arXiv 2024, https://doi.org/10.48550/arXiv.2408.13677

HL 46.5 Thu 10:45 H15

Determination of optical losses at 265 nm in multimode AlGaN waveguides — •Verena Montag[1], Martin Guttmann[2], Bruno Marx[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs) like, e.g., biochemical sensing, solar-blind communication, and UV Raman spectroscopy require materials with a large bandgap energy to enable low optical losses. Currently, no ideal material has been identified that enables low loss waveguides and simultaneously the implementation of active and passive components in the UV spectral range. AlGaN is a promising material which is already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN, especially the absorption losses in AlGaN waveguides have not yet been studied in detail in the UVC spectral range. In this work, 200 μm wide AlGaN waveguides, UV-LEDs, and detectors were monolithically fabricated on AlN/sapphire wafers and the waveguide losses are determined. We were able to measure photocurrents >1 nA using an integrated AlGaN-based photodiode. Also, an exponential decrease of the photocurrent with increasing waveguide length could be observed. However, Monte Carlo ray tracing simulations show that apart from absorption losses in the AlGaN waveguides also scattering losses from surface roughness have to be considered in order to fully explain the results.

15 min. break

Prize Talk HL 46.6 Thu 11:15 H15

Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules — •Annika Janssen — Technische Hochschule Nürnberg — Laureate of the Georg-Simon-Ohm-Prize 2025

Organic photovoltaics (OPV) is one of the emerging solar technologies and has the possibility of more cost-effective and sustainable production compared to conventional silicon cells. The printing technique considered in this thesis is doctor blade printing. In research, this is mainly used to produce OPV, as it is fast and the coating physics is similar to slot-die coating, the technique that is most commonly used for large-scale R2R printing. To produce large modules, a homogeneous coating is important, since the thickness of the layers has an influence on the efficiency of the device. In this work, the influence of the film thickness on the efficiency is investigated experimentally on cell level and the influence of layer thickness variations is studied by means of electrical finite element method (FEM) simulations for large-area modules. Formulas describing the behavior of the injected ink during printing are established. A special focus was put on the analysis of the non-accelerated and the accelerated printing. Using simulations, this work shows that a homogeneous coating achieved by accelerating the doctor blade can improve the efficiency of organic solar modules by 16.22 %.

HL 46.7 Thu 11:45 H15

Ultraflat excitonic dispersion in single layer g-C3N4 — •Francesca Martini, Pietro Nicolò Brangi, Pier Luigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Single-layer graphitic carbon nitride (g-C3N4) is widely regarded as one of the most promising two-dimensional photocatalysts for hydrogen generation via water splitting. Despite its extensive study, limited information is available on its excitonic dispersion and velocity, critical parameters for achieving high charge mobility and efficient photogeneration. In this work, we employ many-body perturbation theory and the Bethe-Salpeter equation to provide a comprehensive description of the optical absorption and finite-momentum energy loss function for both s-triazine and tri-s-triazine structures. Our findings reveal the exciton dispersion and velocity, emphasizing the significant role of localized nitrogen lone pairs in producing remarkably flat excitonic bands with velocities that are two orders of magnitudes smaller than the typical one in two-dimensional materials and of the same order or smaller than the optical phonon frequencies in single layer g-C3N4. As the time-scale for inter-site exciton hopping is longer or similar to a phonon period, our results point to a highly non-conventional exciton propagation.

HL 46.8 Thu 12:00 H15

Investigation of PLD-grown β-CuI — •Aaron Giess, Lukas Trefflich, Gabrielle Benndorf, Marius Grundmann, and Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Copper iodide (CuI) is a transparent semiconductor that is currently of great interest due to its inherent p-type behavior and its high exciton binding energy of 62 meV. Typically, CuI crystallizes in the zincblende structure (γ-CuI) at room temperature. However, CuI can also crystallize in other phases, which are thermodynamically not stable at ambient pressure and temperature. One of these phases is the rhombohedral phase, which is often also called β-phase. Under certain growth conditions, this β-phase appears simultaneously with the γ-phase.

We grew closed thin films of CuI on c-sapphire, using pulsed laser deposition. The influence of the growth-parameters on the occurrence of β-CuI seems to be a multidimensional problem. The most important parameter is the film thickness, with thinner films favouring a higher fraction of the β-phase. The appearance of the β-phase causes additional features in the 2θ-ω scan in XRD, the dielectric function and the optical transmittance. Furthermore, photoluminescence spectra reveal a change of the emission spectra with time, which indicates that a photobleaching processes takes place.

HL 46.9 Thu 12:15 H15

Luminescent Microthermometers Based on ALD-encapsulated Ga_2O_3:Cr DBR Microcavities — •Ruben Neelissen[1], Daniel Carrasco[1,2], Anton Schäning[1], Marco Schowalter[1], Andreas Rosenauer[1], Emilio Nogales[2], Bianchi Mendez[2], Martin Eickhoff[1], and Manuel Alonso-Orts[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-

Allee 1, 28359 Bremen, Germany. — [2]Departamento de Fisica de Materiales, Plaza Ciencias 1, Universidad Complutense de Madrid, 28040 Madrid, Spain.

The ability to measure temperature non-invasively, accurately and reliably is an ever reoccurring challenge in various fields such as micro- and nanosystems. Luminescent thermometry sensors can operate in environments where electronic counterparts are ineffective, thanks to their capability for remote sensing while being minimally intrusive.

Gallium oxide (β-Ga_2O_3) is a semiconductor with an ultra-wide bandgap of 4.8 eV and high resilience. Chromium-Ions (Cr^{3+}) in β-Ga_2O_3 result in two well-defined peaks, superimposed to a red-NIR emission, which can be utilized for temperature sensing.

In this work [1] it is demonstrated how confined light of β-Ga_2O_3:Cr microcavities (MCs) can be enhanced by encapsulating them in ALD-grown distributed Bragg reflectors (DBRs). With increasing temperature, the resonant wavelength redshifts due to changes in both the refractive index and the optical length of the MCs. A temperature accuracy of < 0.5 °C for temperatures above -80 °C is demonstrated.

[1] M. Alonso-Orts et al. In: *Advanced Materials Technologies* (2024), p. 2400881.

HL 46.10 Thu 12:30 H15

Theoretical and Experimental Study of Lead Tungstate (PWO-II) Crystal Properties for Electromagnetic Calorimetry — •Ather Ahmad[1], Pavel Orsich[1], Valera Dormenev[1], Hans-Georg Zaunick[1], Kai-Thomas Brinkmann[1], Simone Sanna[2], Martin Becker[3], and Limei Chen[3] — [1]II. Physikalisches Institut, Gießen, Germany — [2]Institut für Theoretische Physik, Gießen, Germany — [3]I. Physikalisches Institut, Gießen, Germany

Lead tungstate ($PbWO_4$ or PWO) is widely recognized as a high-performance scintillator for electromagnetic calorimeters due to its fast response, high density, and radiation hardness. PWO scintillator material is used in several experiments, such as CMS at the LHC (CERN), and the next-generation PWO-II crystals, which are doped to enhance their properties, have been optimized for the PANDA experiment at FAIR in Darmstadt.

To gain a deeper understanding of the material's performance, we have combined theoretical and experimental approaches to study the electronic and optical properties of PWO-II. Raman spectra and light transmission measurements were conducted on PWO-II samples and compared with results from density functional theory (DFT) calculations. In our models, we consider the crystal phases stable at room temperature, revealing characteristic differences in both Raman spectra and light transmission between these phases.

These combined efforts aim to refine the characterization of PWO-II and support the development of advanced calorimeter materials.

HL 46.11 Thu 12:45 H15

Rabi splitting mediated dual electromagnetically induced transparency in metamaterial — •Amit Haldar[1], Kshitij V Goyal[1], Ruturaj Puranik[2], Vivek Dwij[2], Shriganesh Prabhu[2], and Shovon Pal[1] — [1]NISER, HBNI, Jatni, India. — [2]TIFR, HBNI, Mumbai, India.

Electromagnetically Induced Transparency (EIT) and strong coupling are pivotal phenomena in light-matter interactions with profound implications for quantum and material sciences. EIT, resulting from destructive interference in three-level quantum systems, creates a transparency window within an absorption spectrum [1] and is classically emulated in metamaterials via bright-dark-mode interference. This enables applications such as slow-light devices, sensors, and cloaking technologies. Strong coupling, achieved when the interaction strength between a quantum emitter and an electromagnetic field surpasses system losses, leads to hybridized states (Rabi splitting), facilitating coherent energy exchange and insights into coupling mechanisms [2]. This study combines these phenomena using terahertz metamaterials to achieve tunable transitions between single and dual EIT states through strong coupling. This integration enhances the tunability of metamaterial-based devices and deepens our understanding of EIT and strong coupling, bridging classical and quantum perspectives for future applications.

[1] S. Y. Chiam *et al.*, *Phys. Rev. B* **80**, 153103 (2009).
[2] H. S. Kim *et al.*, *Nano Lett.* **20**, 6690 (2020).

HL 47: Focus Session: Quantum Technologies in Deployed Systems II

Recent advancements in quantum cryptography, quantum computing, and quantum sensing are driving researchers to develop a universal quantum network*known as the quantum internet, which will enable secure connections among quantum computers, as well as to networks of quantum sensors, through quantum cryptography. Building a functional quantum internet is one of the most ambitious goals in quantum technology for the coming decades.

The focus sessoin aims to provide a comprehensive overview of the corresponding platforms and advances in quantum technologies, and is organized by Simone L. Portalupi (U. Stuttgart), Michal Vyvlecka (U. Stuttgart) and Michael Zopf (U. Hannover).

Time: Thursday 9:30–12:30 Location: H17

Invited Talk HL 47.1 Thu 9:30 H17

Quantum-Dot Quantum Light Sources in Deployed Systems — •Peter Michler — Institute for Semiconductor Optics and Functional interfaces, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany

Quantum photonic networks require sources of single, indistinguishable and entangled photon pairs with high brightness [1]. Semiconductor quantum dots (QDs) hold great promise to meet these requirements. In many foreseen implementations of quantum photonic networks, full-photonic quantum teleportation is a cornerstone, and the photons must be able to propagate over long distances in silica fibers with limited absorption and wave packet dispersion. Photons in the so-called telecom bands will experience minimum absorption (C-band) and dispersion (O-band). Moreover, from a practicable point of view, portable rack single- and entangled photon sources are advantageous in deployed systems.

In this talk, we report on the performance of quantum-dot quantum light sources in deployed fibers [2], and demonstrate quantum teleportation with telecom photons from remote quantum emitters [3]. Moreover, QKD with entangled photons is demonstrated in deployed fibers and the performance of a QD based portable rack single- and entangled photon source, which can be operated down to 4 K, is presented.

References: [1] R. Joos et al., Nano Letters 24, 8626 (2024) [2] T. Strobel et al., Optica Quantum 2, 274 (2024) [3] T. Strobel et al., arXiv:2411.12904 (2024)

Invited Talk HL 47.2 Thu 10:00 H17

Field test of semiconductor quantum light sources — •Fei Ding — Leibniz University Hannover, Germany

Semiconductor quantum dots (QDs) are among the most promising quantum light sources, with the potential to revolutionize quantum communication research. For instance, utilizing on-demand single photons and entangled photons in quantum key distribution (QKD) protocols can significantly enhance security and increase the maximum tolerable loss. However, several critical challenges must be addressed to bridge the gap between laboratory experiments and long-distance field tests using QDs. In this talk, I will first review our work over the past years on QD-based single-photon and entangled-photon sources. Following that, I will present our recent field tests of single photon transmissions over a 79 km link between Hannover and Braunschweig, with 25.49 dB loss, equivalent to 130 km in direct-connected optical fiber.

Invited Talk HL 47.3 Thu 10:30 H17

Quantum dot based quantum communication in urban networks — •Rinaldo Trotta — Sapienza University of Rome, Italy

The last two decades have witnessed an impressive progress in the development of single and entangled photon sources based on quantum dots. It has now arrived the moment to explore their full potential in urban quantum-communication scenarios.

In this talk, I will first discuss how single and entangled photons generated by quantum dots can be used to implement advanced quantum communication protocols in a controlled laboratory environment. Then, I will show our efforts towards the construction of a hybrid quantum network, harnessing both fibre and free-space links, within the University campus in the centre of Rome. Finally, I will present field demonstrations of point-to-point entanglement-based quantum key distribution and three-node quantum teleportation with dissimilar quantum dots. A discussion on future challenges and perspectives will conclude the talk.

15 min. break

Invited Talk HL 47.4 Thu 11:15 H17

Quantum communication protocols over a 14-km urban fiber link — •Jürgen Eschner — Universität des Saarlandes, Experimentalphysik, 66123 Saarbrücken, Germany

Quantum communication over urban telecom fibers poses challenges such as environmentally induced polarization fluctuations and lossy splices. We report on the characterization and operation of a 14-km long fiber link across Saarbrücken for quantum communication. The dark fiber has underground and overground sections and $\sim 9\,\mathrm{dB}$ attenuation. We stabilize its polarization with $> 99\%$ process fidelity up to 60 s. For implementing quantum communication protocols we employ a $^{40}Ca^{+}$ single-ion quantum memory, an ion-resonant entangled photon-pair source, and quantum frequency conversion.

We distribute photonic entanglement without significant fidelity degradation. Using heralded absorption of one photon of the entangled pair, we also demonstrate atom-to-photon quantum state teleportation over the fiber link with $\sim 84\%$ average fidelity [1].

In a laboratory experiment we also realize a quantum repeater cell based on two $^{40}Ca^{+}$ ions that are asynchronously entangled with their emitted photons. By entanglement swapping via a Mølmer-Sørensen quantum gate on the ions, which are located in the same trap, we generate photon-photon entanglement with $\sim 76\%$ average fidelity [2].

[1] S. Kucera et al., npj Quantum Information **10**, 88 (2024)
[2] M. Bergerhoff et al., Phys. Rev. A **110**, 032603 (2024)

HL 47.5 Thu 11:45 H17

Quantum cryptography at deployed communication networks with quantum dots at telecommunication wavelengths — •Anna Friederike Köhler[1], Tim Strobel[1], Michal Vyvlecka[1], Raphael Joos[1], Ilenia Neureuther[1], Timo Schnieber[1], Tobias Bauer[2], Marlon Schäfer[2], Nand Lal Sharma[3], Weijie Nie[3], Ghata Bhayani[3], Caspar Hopfmann[3], Simone Luca Portalupi[1], Christoph Becher[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Campus E2.6, 66123 Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Quantum cryptography leverages quantum effects to achieve unprecedented security. Quantum dot-based nonclassical light sources hold a promise for efficient cryptographic applications, offering on-demand generation of entangled photon pairs with high brightness and negligible multi-photon contribution. These features enable high-speed quantum communication while minimizing security risks. In this work, we demonstrate the BBM92 quantum key distribution protocoll using a GaAs quantum dot source to produce high-fidelity entangled photon pairs. Frequency conversion to telecommunication wavelengths is implemented to enhance transmission efficiency in a deployed intracity silica-based fiber network.

HL 47.6 Thu 12:00 H17

Experimental Quantum Strong Coin Flipping using a Deterministic Single-Photon Source — Daniel Vajner[1], •Koray Kaymazlar[1], Fenja Drauschke[2], Lucas Rickert[1], Martin von Helversen[1], Shulun Li[3], Zhichuan Niu[3], Anna Pappa[2,4], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technische Univeristät Berlin, Germany — [2]Electrical Engineering and Computer Science Department, Technische Univeristät Berlin, Germany — [3]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [4]Fraunhofer Institute for Open Communication Systems - FOKUS, Technical University Berlin, Germany

Strong coin flipping (SCF) is a fundamental cryptographic protocol allowing two distrustful parties to agree on randomly generated bit. In this work, we report the first implementation of a quantum strong coin flipping protocol that yields a quantum advantage compared to both its classical counterpart and an implementation using weak coherent pulses.

The quantum advantage is enabled by employing a state-of-the-art deterministic single-photon source based on a quantum dot embedded in a high-Purcell microcavity. Using a fiber-based electro-optic modulator (EOM) in single-pass configuration in combination with a self-built arbitrary waveform generator we realize fast dynamic, random polarization-state encoding at 80 MHz clock-rate.

Our QSCF implementation enables a coin flipping rate of 1.5 kHz and an average quantum bit error ratio (QBER) below 3%, sufficient to realize a quantum advantage.

HL 47.7 Thu 12:15 H17

Establishing a Quantum Local Area Network in Berlin City using Deterministic Quantum Light Sources — •Martin von Helversen[1], Lucas Rickert[1], Anne Rohwäder[1], Kinga Zolnacz[2], Koray Kaymazlar[1], Daniel Vajner[1], Anna Musial[3], Grzegorz Sek[3], Hanqing Liu[4], Zhichuan Niu[4], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technical University Berlin, Berlin, Germany — [2]Department of Optics and Photonics, Wroclaw University of Science and Technology, Wroclaw, Poland — [3]Department of Experimental Physics, Wroclaw University of Science and Technology, Wroclaw, Poland — [4]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China

Applications of quantum information enabled by solid-state quantum light sources currently witness the transition from laboratory proof-of-concept to field-experiments. In this contribution we present our recent progress in establishing a quantum local area network at the Campus Charlottenburg of TU Berlin. We show results of an actively stabilized free-space optical link with an effective length of 400 m and an end-to-end transmission of >70%. In addition, we operate a fiber-link between two buildings consisting of 6x 650 m of dark optical fiber. Moreover, we discuss the deployment of mobile deterministic single-photon sources based on compact cryocoolers and fiber-pigtailed quantum dot microcavities [FC-CBG] and evaluate the suitability for implementations of different types of cryptographic primitives. [1] Rickert, Lucas, et al., arXiv:2409.08982 (2024) [2] Rickert, Lucas, et al., arXiv:2408.02543 (2024).

HL 48: Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)

Superconducting monolayer transition metal dichalcogenides (TMDs) like $NbSe_2$, TaS_2, and gated WSe_2 or MoS_2, have attracted lot of interest in recent years. On the one hand Ising spin-orbit coupling pins the electron's spin out of plane, and hence is responsible for critical in-plane magnetic fields by far exceeding the Pauli limit. On the other hand, while the underlying pairing mechanism is still under debate, recent experiments provide strong evidence for its unconventional, multiband, nature. The Focus Session will feature experimental and theoretical advances on the superconductivity in monolayer TMDs, with focus on universal features, a possible Luttinger-Kohn mechanism, a nodal or even chiral nature of the gap functions, and their phase diagram.

Organizers: Milena Grifoni (Universität Regensburg), Julian Siegl (Universität Regensburg)

Time: Thursday 9:30–12:45 Location: H36

Topical Talk HL 48.1 Thu 9:30 H36

Evidence of Unconventional Superconductivity in Monolayer and Bulk van der Waals Material TaS_2 — •Somesh Chandra Ganguli[1], Viliam Vano[1,2], Yuxiao Ding[1], Maryam Khosravian[1], Jose Lado[1], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University FI-00076 Aalto, Finland — [2]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, NJ, USA

Unconventional superconductors are at the forefront of modern quantum materials' research. Even though unconventional superconductivity has been discovered in a large number of bulk systems, intrinsic unconventional superconductivity in the monolayer limit has remained elusive.

In our work, we demonstrate the evidence of nodal f-wave superconductivity in monolayer 1H-TaS_2. We also observe the emergence of many-body excitations potentially associated to its unconventional pairing mechanism. Furthermore, the nodal f-wave superconducting state in the pristine monolayer 1H-TaS_2 is driven to a conventional gapped s-wave state by the inclusion of non-magnetic disorder. I will also briefly describe our recent results on bulk layered superconductor 6R-TaS_2 where alternating metallic and Mott insulating layers gives rise to unconventional superconductivity.

Our results demonstrate the emergence of unconventional superconductivity in van der Waals (vdW) materials and therefore opens possibilities to create designer unconventional superconductivity in vdW heterostructures.

Topical Talk HL 48.2 Thu 10:00 H36

Signatures of Unconventional Superconductivity in Transition Metal Dichalcogenides — •Miguel Ugeda — Donostia International Physics Center, San Sebastián, Spain

Lowering the dimensionality of a material is an effective strategy to boost electronic correlations that fail to be captured by conventional pictures. In this arena, two-dimensional (2D) materials provide an ideal platform for the exploration of quantum collective phenomena arising from such strong interactions due to their simple synthesis and modelling. In this talk, I will review the rich physics that emerges in the family of transition metal dichalcogenide (TMD) metals in the superconducting state in the 2D limit. While many of these TMD metals exhibit superconductivity in both the bulk form down to the monolayer, the latter limit stores exciting surprises beyond the BCS frameworks that have been revealed in the last years. I will focus on our $NbSe_2$, the most representative TMD superconductor, where I will describe our recent STM/STS experiments. Lastly, I will briefly describe our current efforts to induce unconventional superconductivity in more complex TMD heterostructures.

Topical Talk HL 48.3 Thu 10:30 H36

Friedel Oscillations and Chiral Superconductivity in Monolayer $NbSe_2$ — •Magdalena Marganska[1,2], Julian Siegl[1], Anton Bleibaum[1], Marcin Kurpas[3], Wen Wan[4], John Schliemann[1], Miguel M. Ugeda[4,5], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93 053 Regensburg — [2]Institute for Theoretical Physics, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland — [4]Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao 48013, Spain

In 1965 Kohn and Luttinger proposed a mechanism for superconductivity, based on the electronic Coulomb interaction alone. The screening effects, which cause Friedel oscillations of charge density around impurities, modulate also the interaction between moving electrons. If it has attractive regions, superconductivity can arise by exploiting them. This mechanism, negligible in 3D metals, can become much stronger in 2D electronic systems. In a monolayer of $NbSe_2$ the screening is further suppressed, due to the multi-orbital nature of the electronic band at the Fermi level. We show how this, and the presence of K/K' Fermi surfaces, leads to superconducting pairing. The dominant gap solution at $T = 0$ has the chiral p+ip symmetry. It evolves with increasing temperature, turning from fully chiral at T=0 to a nematic solution with p-like symmetry close to the critical temperature. Our results are also consistent with our tunneling spectroscopy measurements in $NbSe_2$.

15 min. break

Topical Talk HL 48.4 Thu 11:15 H36

Unconventional Pairing in Ising Superconductors — •Andreas Kreisel[1], Subhojit Roy[2,3,4], Brian M. Andersen[1], and Shantanu Mukherjee[2,3,4] — [1]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [2]Department of Physics, Indian Institute of Technology Madras, Chennai, 600036, India — [3]Center for Atomistic Modelling and Materials Design, IIT Madras, Chennai 600036, India — [4]Quantum Centers in Diamond and Emergent Materials (QCenDiem)-Group, IIT Madras, Chennai, 600036 India

Ising spin orbit coupling arises in materials with non-centrosymmetric crystal structure in conjunction of an in-plane mirror symmetry and is realized in some two dimension transition metal dichalcogenides. Example materials are monolayer $NbSe_2$, MoS_2, TaS_2, and $PbTe_2$, where signatures of unconventional superconductivity are found in contrast to their three dimensional bulk counterparts. In this talk, I present a microscopic formalism to calculate the superconducting instability from a momentum-dependent spin- and charge-fluctuation-mediated pairing interaction in presence of spin orbit coupling that induces a spin splitting. This pairing is then applied to the electronic structure of transition metal dichalcogenides. We provide a quantitative measure of the mixing between the even- and odd-parity superconducting states which varies with Coulomb interaction. The pairing scenario from spin fluctuations together with the mixing of the odd-parity superconducting state gives rise to an enhancement of the critical magnetic field.

Topical Talk HL 48.5 Thu 11:45 H36

High-Field Study of Ising Superconductivity in TMDs — •Oleksandr Zheliuk[1,2], Xiaoli Peng[3], Andrew Ammerlaan[1,2], Puhua Wan[3], Yulia Kreminska[3], Steffen Wiedmann[1,2], Uli Zeitler[1,2], and Jianting Ye[3] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, Nijmegen 6525 ED, The Netherlands — [2]Radboud University, Institute for Molecules and Materials, Nijmegen 6525 AJ, The Netherlands — [3]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands

Semiconducting transition metal dichalcogenides are known for their strong spin-orbit coupling, the possibility of hosting a variety of quantum phases such as two-dimensional superconductivity with upper critical fields that by far bypasses the Pauli limit, Josephson coupled

states, and high mobility electron gasses accessed in electric double-layer transistor (EDLT) configuration. Despite its well-established electronic structure, the dome-shaped superconducting phase diagram where the critical temperature T_c can be modulated by carrier concentration is yet to be understood. This talk will sharpen the understanding of the electronic structure of the electron-doped MoS_2, covering recent insights into superconductivity in MoS_2 probed via the multivalley transport phenomena accessed in high magnetic field.

HL 48.6 Thu 12:15 H36

Unconventional Pairing in Ising Superconductors: Application to Monolayer $NbSe_2$ — •Subhojit Roy[1], Andreas Kreisel[2], Brian Andersen[3], and Shantanu Mukherjee[4] — [1]Indian Instititute of Technology Madras, Chennai, 600036, India — [2]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [3]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [4]Indian Instititute of Technology Madras, Chennai, 600036, India

The presence of a non-centrosymmetric crystal structure and in-plane mirror symmetry allows an Ising spin-orbit coupling to form in some two-dimensional materials, where a nontrivial nature of the superconducting state is currently being explored. In this study(1), we develop a microscopic formalism for Ising superconductors that captures the superconducting instability arising from a momentum-dependent spin- and charge-fluctuation-mediated pairing interaction. We apply our pairing model to the electronic structure of monolayer $NbSe_2$, where first-principles calculations reveal the presence of strong paramagnetic fluctuations. Our calculations provide a quantitative measure of the mixing between the even- and odd-parity superconducting states and its variation with Coulomb interaction. Further, numerical analysis in the presence of an external Zeeman field reveals the role of Ising spin-orbit coupling and mixing of odd-parity superconducting state in influencing the low-temperature enhancement of the critical magnetic field.

[1] S. Roy et al., 2D Mater. 12 015004 (2025).

HL 48.7 Thu 12:30 H36

Emergence of Unconventional Superconductivity and Doped Mott Physics in 6R-TaS_2 — •Yuxiao Ding[1], Amritroop Achari[2], Jonas Bekaert[3], Jose Lado[1], Rahul R. Nair[2], Peter Liljeroth[1], and Somesh C. Ganguli[1] — [1]Aalto University, Finland — [2]University of Manchester, UK — [3]University of Antwerp, Belgium

Discovery of Unconventional superconductivity in van der Waals (vdW) materials have brought about a paradigm shift in modern condensed matter research for their tunability and potential application in quantum computing. Among these, most prevalent are 4Hb-TaS_2 and 6R-TaS_2. They comprise of alternating Mott insulating and metallic layers and give rise to exotic quantum states such as topological superconductivity, anomalous Hall effect potentially associated with hidden magnetism etc. We have studied, using low temperature STM/STS, the newly discovered vdW superconductor 6R-TaS_2. For the 1T phase, a doped Mott phase was observed with potential charge order occurring due to hybridisation between 1T and underlying 1H layer. We also observe Kondo sites in the half-filled regime, which unlike 4Hb-TaS_2, were more robust under the application of tip-induced electric field. This indicates significantly different interlayer interactions in these two systems. We also observe evidence of unconventional superconductivity in the 1H phase, indicated by the presence of V-shaped superconducting gap and many-body excitations. Our results pave a new direction in understanding the role of interplay between magnetism and superconductivity in layered unconventional superconductors.

HL 49: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

HL 49.1 Thu 10:30 H11

Charge ordered phases in the hole-doped triangular Mott insulator 4*Hb*-TaS_2 — •Byeongin Lee[1], Junho Bang[1], Hyungryul Yang[1], Sunghun Kim[2], Dirk Wulferding[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, Ajou University, Suwon 16499, Republic of Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Republic of Korea

4*Hb*-TaS_2 has a unique layered structure, featuring a heterojunction between a 2D triangular Mott insulator and a charge density wave metal. Since a frustrated spin state in the correlated insulating layer is susceptible to charge ordering with carrier doping, it is required to investigate the charge distribution driven by interlayer charge transfer to understand its various phases. In this study, we utilize scanning tunneling microscopy and spectroscopy (STM/S) to examine the charge-ordered phases of 1*T*-TaS_2 layers within 4*Hb*-TaS_2, explicitly focusing on the non-half-filled regime. Our STS findings reveal an energy gap that exhibits an out-of-phase relation of the charge density. We attribute the emergence of the charge-ordered insulating phase in a doped triangular Mott insulator to the interplay between on-site and nonlocal Coulomb repulsion.

HL 49.2 Thu 10:45 H11

Superlattice engineering in graphene and 1T-$NbSe_2$ heterostructures — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I. Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering has become a major branch of condensed matter research, not at least due to the variety of exotic states observed twisted in van der Waals heterostructures. We here present a new method to periodically modulate graphene by stacking it on 1T/2H-$NbSe_2$. By tuning the twist angle, we realized two near-commensurate superlattices: $\sqrt{3}\times\sqrt{3}$ and 2×2 aligned with the charge density wave (CDW) of 1T-$NbSe_2$. Using scanning tunnelling microscopy, we visualized local stacking configurations for these two superlattices. We applied a newly developed symmetry analysis method to track rotational symmetry breaking as a function of bias. In the 2×2 superlattice, C_3 rotational symmetry was preserved. However, in the $\sqrt{3}\times\sqrt{3}$, a strong strip phase occurs. This symmetry breaking is explained by our tight-binding model. Our findings highlight a mechanism for superlattice-induced symmetry breaking that hints towards exotic states of matter.

HL 49.3 Thu 11:00 H11

Influence of Edge Termination on the Electronic Structure of Single Layer MoS_2 on Graphene/Ir(111) — •Alice Bremerich[1], Marco Thaler[2], Thais Chagas[1], Borna Pielic[1], Laerte Patera[2], and Carsten Busse[1] — [1]Universität Siegen, Deutschland — [2]Universität Innsbruck, Österreich

MoS_2 is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic edge state that induces partial charge accumulation at its edges, resulting in band bending effects. This 1D state acts as a barrier to electron transport across the edge and contributes significantly to quantum confinement effects in TMDC islands. In this study, we tune the edge state and the associated band bending by altering the edge termination of MoS_2/gr/Ir(111) and investigate the resulting changes in the electronic structure by Scanning Tunneling Microscopy and Spectroscopy (STM and STS) at 8 K.

Quasi-freestanding MoS_2 is grown on gr/Ir(111) by Molecular Beam Epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). We vary the chemical potential of sulfur and thereby modify the chemical environment of the boundaries. The partial charge at the perimeter depends on edge type as well as edge chemistry. In consequence, also the upward bending of both valence and conduction band shows distinct variations.

HL 49.4 Thu 11:15 H11

magnetic-field-induced dimensionality transition of charge density waves in strained 2H-NbSe2 — •Ryo Ichikawa[1], Yukiko Takahashi[2], Eiichi Inami[3], and Toyo Kazu Yamada[1,4] — [1]Department of Material Science, Chiba University — [2]National

Institute for Material Science, Tsukuba — [3]School of system Engineering, Kochi University of Technology — [4]Molecular Chirality Research center, Chiba University

Layered transition metal dichalcogenides (TMDs) exhibit various correlated phases, including charge density waves (CDW), superconductivity, and magnetic orders. Bulk 2H-NbSe2 (2H niobium diselenide) is one of the most extensively studied TMDs, showing a triangular (3Q) incommensurate CDW with a 3a period in real space (3 * 3, TCDW ~ 33 K). Electric and magnetic fields have been used to manipulate spatial or time inversion symmetry, while the CDW in 2H-NbSe2 remains robust even under large magnetic fields on the order of tens of Tesla. However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe2, where a weak magnetic field of approximately 30 mT can switch the electronic phase within the thin film, resulting in a supercurrent diode effect. This study investigates the strained 2H-NbSe2 exhibiting the 2*2 CDW phase. We utilize low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) in ultrahigh vacuum (UHV). STS maps reveal the coherence of the 2*2 CDW patterns. However, applying an out-of-plane magnetic field induces a dramatic transformation akin to that observed in 1T-NbSe2, shifting the metallic 2D CDW pattern to a 1D CDW pattern.

HL 49.5 Thu 11:30 H11

Ultrafast phonons dynamics of monolayer transition metal dichalcogenides — •yiming pan and fabio caruso — Kiel University, Germany

Valley degrees of freedom in transition-metal dichalcogenides influence thoroughly electron-phonon coupling and its nonequilibrium dynamics. Here we present a time-resolved ab-initio study of the ultrafast dynamics of chiral phonons following carrier excitation with circularly-polarized light. By investigating the valley depolarization dynamics of monolayer MoS_2 and WS_2, we find that a population imbalance of carriers distributed at K and K′ can lead to valley polarized phonons persisting beyond 10 ps, and characterized by a distinctive chirality [1]. Additionally, we find that strain can be exploited as a tool to control the phonon emission and the relaxation channels of hot carriers [2]. Finally, we briefly discuss available opportunities for experimental detection of these phenomena

[1] Y. Pan and F. Caruso, Nano Lett. 23, 7463 (2023)
[2] Y. Pan and F. Caruso, npj 2D Mater. Appl. 8, 42 (2024)

HL 49.6 Thu 11:45 H11

Probing Excitonic Properties and Structural Effects in WS_2-Graphene Heterostructures Using EELS and DFT-BSE Modeling — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Robin Günkel, Badrosadat Ojaghi Dogahe, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the excitonic properties of WS_2 epitaxially grown on graphene by metal-organic chemical vapor deposition. We focus on understanding the effects of structural changes, such as variations in the number of WS_2 layers. Using monochromatic electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), we observe in the monolayer region of WS_2 an excitonic spectrum with excitonic peaks at 2.0 eV and 2.4 eV, as well as additional spectral features at higher energies. Measurements in the bilayer region show a small redshift of these features due to the additional layer. Complementary density functional theory and Bethe-Salpeter calculations show that this redshift in the K-valley excitons is due to both a change in quantum confinement and a change in the WS_2 lattice constant, with the latter being the dominant effect. Using STEM, this lattice distortion can be attributed to the heteroepitaxial alignment of the lower WS_2 layer to the graphene substrate, while the upper layer is relaxed. This study provides valuable insights into the relationship between atomic structure and optical properties in complex material systems, providing essential knowledge for the design and optimization of 2D heterostructures for advanced device applications.

HL 49.7 Thu 12:00 H11

Optical excitations in 2H-MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Münster, Institute of Physics and Center for Nanotechnology, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Theoretical and experimental investigations have shown several changes in the optical spectrum of the 2H-MoS_2 bilayer under pressure [1].

By using density functional theory (DFT) and many-body perturbation theory in combination with linear elasticity, our computational investigations show an effective shift of the A exciton under pressure. It is strongly connected to the behavior of the direct band gap at the K point, which shifts in energy under pressure. The direction of this shift depends on the stress condition. While a hydrostatic pressure leads to a blueshift, a suppression of the in-plane contraction, as it appears in diamond anvil cell-experiments due to the interaction between the sample and the substrate, shows a redshift.

Moreover, we observe a similar behavior for the interlayer exciton, whereas the shift rate is smaller than that of the A exciton, which results in a decreasing A-IL splitting for an increasing pressure.

[1] P. Steeger, J. Graalmann et al., Nano Lett., 23, (2023)

HL 49.8 Thu 12:15 H11

Visualizing and controlling charge states of metal nanoislands on a two dimensional semiconductor — •Junho Bang[1], Byeongin Lee[1], Jian-Feng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul, Korea — [2]Department of Topological Quantum Chemistry, Max Planck Institute for Chemical Physics of Solids, München ,Germany

Nanoscale objects show unique electronic behaviors when weakly coupled to electrodes. Coulomb blockade (CB) can occur in such systems, where the repulsive Coulomb interaction between electrons prevents additional electrons from entering the quantum dots, hindering their flow. Single electron tunneling occurs by these correlated electron transports, leading to the discrete charge states of objects in double barrier tunneling junctions. Despite enormous progress, challenges remain in precisely controlling the interplay between objects' charge states and tunneling dynamics under varying conditions. Here, we visualize the charge states and their spatial variation on the random array of the indium islands on two-dimensional semiconductor black phosphorus using scanning tunneling microscopy and spectroscopy. Our spatially resolved tunneling spectra reveal that the junction capacitance varies across the islands. Furthermore, we find that the CB features are visible outside the islands, which is attributed to the remote gating of the islands. Our work advances the manipulation of electron transport at the nanoscale, which will be helpful in the application of nanoscale object-based single-electron devices.

HL 50: 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Thursday 15:00–17:45 Location: H6

HL 50.1 Thu 15:00 H6

Systematic Study of Interlayer Interactions in Transition Metal Dichalcogenide Bilayers Using microARPES — •Thomas Nielsen[1], Chakradhar Sahoo[1], Alfred Jones[1], Zhihao Jiang[1], Kenji Watanabe[2], Takashi Taniguchi[2], Suman Chakraborty[4], Prasana Sahoo[4], Jill A. Miwa[1], Yong P. Chen[1,3], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan — [3]Department of Physics, Purdue University, USA — [4]Materials Science Centre, Indian Institute of Technology, India

Stacked transition metal dichalcogenide monolayers are emerging as a platform to study correlated phases such as Mott insulators or Wigner crystallization. Spatially resolved ARPES can potentially visualize the moiré bands and hybridization effects in the electronic structure underpinning these correlated phases. Observing these phenomena in ARPES in a reproducible way remains challenging, motivating systematic studies of interlayer interactions in twisted TMD bilayers. 20 different heterobilayers of WSe_2, WS_2, $MoSe_2$, and WS_2, as well as homobilayers of WSe_2 are fabricated with varying twist angles. Their electronic properties are measured using the microARPES branch at the ASTRID2 synchrotron at Aarhus University. Band alignments and hybridization effects are tracked as a function of material composition and twist angle. The used dry-transfer fabrication techniques do not yield the direct observation of flat bands from moiré effects in the valence band. Based on this work future avenues for reproducibly attaining moiré effects in photoemission from TMDs are discussed.

HL 50.2 Thu 15:15 H6

Gate-Tunable miniband dispersion in twisted graphene superlattices near the magic angle measured with MicroARPES — •Alfred J. H. Jones[1], Zhihao Jiang[1], Dongkyu Lee[2], Youngji Park[2], Kimberly Hsieh[1], Paulina Majchrzak[1], Chakradhar Sahoo[1], Thomas S. Nielsen[1], Kenji Watanabe[3], Takashi Taniguchi[3], Philip Hofmann[1], Jill A. Miwa[1], Yong P. Chen[1,4], Jeil Jung[2], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, University of Seoul, Korea — [3]National Institute for Materials Science, Japan — [4]Department of Physics and Astronomy, Purdue University, USA

Twisted superlattices of mono- and bilayer-graphene are emerging as powerful tools to explore quantum many-body effects such as unconventional superconductivity and Mott insulating states. Access to the momentum-resolved electronic structure simultaneous to changing the carrier concentration and displacement field within a twisted superlattice device can directly provide key information on the miniband dispersion tunability that underpins the correlated phenomena.

Here, we present microARPES measurements from SGM4 at ASTRID2 on two-terminal "near-magic-angle" twisted bilayer (TBG) and double-bilayer graphene (TDBG) devices. Our findings for the two systems are strikingly different: On TBG, we find a filling factor-dependent bandwidth change of the flat moiré bands, whereas on TDBG the effect of tuning the doping and displacement field leads to non-monotonous bandwidth changes and tunable gap opening effects.

HL 50.3 Thu 15:30 H6

Topological magnetic Moiré heterostructures — •Aymeric Saunot[1,3], Sebastien E. Hadjadj[2], Tonica Valla[1], Maxim Ilyn[3], and Ilya I. Klimovskikh[1] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastían, Basque Country, Spain. — [2]Materials Physics Center (MPC), Paseo Manuel de Lardizabal N5,b20018 Donostia, Spain. — [3]Departamento de Física de Materiales UPV/EHU, San Sebastían, Spain.

Over the last few years Moiré superlattices have become a hot topic in condensed matter, thanks to the experimental success of magic angle twisted graphene. Moiré superpotentials arise from either twist or atomic mismatch at the interface between van der Waals materials, leading to a rich physics of strongly correlated electrons. Intriguingly, creation of Moiré pattern on the surface of 3D topological insulator (TIs) is theoretically expected to lead to, among others, topological superconductivity, high Chern number systems and non-trivial magnetic textures. Here, we present Moiré heterostructures made from 3D TIs and novel 2D magnetic insulators transition metal dihalides. We investigate the heterostructure's surface by means of STM, ARPES, XMCD, and LEED. Our results show that the Moiré periodicity and the symmetry of the potential, can be tuned based on the ratio between the lattice parameters of the heterostructure's layers. Band structure measurements excitedly show the main Dirac cone surrounded by several Dirac cone replicas creating new Dirac minicones at the crossing points, opening a whole new platform to study topological Moiré physics.

HL 50.4 Thu 15:45 H6

SNOM of lateral TMDC heterojunctions — •Philipp Schwendke[1], Samuel Palato[1], and Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG

Two transition metal dichalcogenide monolayers, joined together laterally, form a one-dimensional heterojunction where charge transfer with associated space charge region and current rectification have been shown experimentally [1]. Furthermore, there are unique local electronic properties determining the excitonic response in the boundary region. Nanoscale spectroscopic methods are needed for the observation of such local optical properties. We use scanning near-field optical microscopy (SNOM) in combination with a continuous wave (cw) light source at 633 nm, as well as a pulsed laser tunable in a wide range from 250 nm to 1300 nm. We employ pseudo-heterodyne modulation for noise suppression and optical phase information, and quadrature-assisted discrete demodulation in order to use the tunable light source at kHz repetition rates. Resonant SNOM measurements show a quenching near the WS_2-MoS_2 boundary, which can be indicative of local energy shifts or electronic states specific to the boundary region. This is complementary to previous measurements which show quenching of photoluminescence [2], attributing it to exciton recombination. In addition, the agreement of results acquired with cw and pulsed light sources paves the way towards time-resolved near-field measurements.

[1] Li et al., Science, vol 349, p 524 (2015)
[2] Chou et al., Nanoscale, vol 14, p 6323 (2022)

HL 50.5 Thu 16:00 H6

Charge density wave interactions in bilayer 1T-TaSe2 — •Robert Drost, Ziying Wang, Büşra Arslan, Adolfo Fumega, Jose Lado, and Peter Liljeroth — Aalto University, Department of Applied Physics

Van der Waals materials offer splendid opportunities for quantum material engineering through stacking and heterostructure formation. While well-proven for many essential two-dimensional materials, these techniques are less explored for correlated materials. The 1T phase of TaSe2 is a two-dimensional Mott insulator and and excellent model system for correlations in reduced dimensions. The correlation gap in 1T-TaSe2 is highly sensitive to the thickness of the material, suggesting that electron-electron interactions between the charge density waves play an important role in determining the electronic properties of few-layer TaSe2. We also observe and additional site dependence of the gap size, showing that the stacking order may be equally important. These effects hint at the possibility of using charge density wave stacking as a design element in new quantum materials.

HL 50.6 Thu 16:15 H6

Giant Zeeman effect at a magnetic topological van der Waals interface — Tobias Wichmann[1,2], Keda Jin[1,3], Jose Martinez-Castro[1,3], Tom G. Saunderson[4,5], Honey Boban[6], Lukasz Plucinski[6], Yuriy Mokrousov[4,5], Markus Ternes[1,3], F. Stefan Tautz[1,2], and •Felix Lüpke[1,7] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]Institut für Experimentalphysik IV A, RWTH Aachen University — [3]Institut für Experimentalphysik II B, RWTH Aachen University — [4]Institute of Physics, Johannes Gutenberg University Mainz — [5]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich — [6]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [7]II. Physikalisches Institut, Universität zu Köln

We report giant Zeeman effects with Landé g-factors up to $g \approx 230$ at the interface of graphene and the van der Waals (vdW) ferromagnet Fe_3GeTe_2 (FGT). They arise from orbital moments generated by the non-trivial band topology of the FGT and cause a huge asym-

metric level splitting when a magnetic field is applied. By exploiting the inelastic phonon gap of graphene, we can directly access the vdW interface to the FGT underneath by scanning tunnelling microscopy and spectroscopy. By analyzing the Faraday-like screening of the tunnelling tip by the graphene, we are able to quantify the electric field at the vdW interface.

HL 50.7 Thu 16:30 H6

Nanoscale band-gap modulation and dual moiré superlattices in the weakly-coupled h-BN/graphite heterostructure — Fábio J. R. Costa[1,2], Luiz F. Zagonel[1], Tin S. Cheng[3], Jonathan Bradford[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergei V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Klaus Kuhnke[2], Klaus Kern[2,6], and •Anna Rosławska[2] — [1]Unversity of Campinas, Brazil — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Nottingham, United Kingdom — [4]Laboratoire Charles Coulomb, Montpellier, France — [5]Institut Universitaire de France, Paris, France — [6]EPFL, Lausanne, Switzerland

Van der Waals materials, such as hexagonal boron nitride (h-BN), and their heterostructures are highly promising for novel nanophotonic and electronic devices. In such stacks, moiré patterns arise and modulate the electronic properties of the material at the scale of typical superstructure periods (approx. 10 nm), and as such are challenging to probe. Here, we investigate the moiré superlattices in the weakly coupled h-BN/graphite heterostructure at the atomic scale. Scanning tunneling microscopy (STM) imaging reveals extensive moiré unit cells on the surface, while spectroscopic measurements demonstrate significant modulation in the work function and band gap across the periodic supercell. Additionally, we identify a dual moiré superlattice in twisted bilayers of h-BN on graphite, providing an extra degree of freedom to tune the heterostructure's properties.

HL 50.8 Thu 16:45 H6

Impact of point defects and grain boundaries on sulfur diffusion and memristive properties of MoS_2 single sheets — •Aaron Flötotto[1], Jules Oumard[1], Benjamin Spetzler[2], Martin Ziegler[2], Erich Runge[1], and Christian Dressler[1] — [1]Technische Universität Ilmenau, Germany — [2]Christian-Albrechts-Universität zu Kiel, Germany

The memristive properties of transition metal dichalcogenides, such as MoS_2, are currently the subject of intense research and have recently been traced back to the dynamics of sulfur vacancies [1, 2]. In this theoretical work, we employ molecular dynamics to determine the sulfur vacancy diffusion coefficients in the vicinity of various point defect structures and grain boundaries in single sheet MoS_2. To address the necessity of large cell sizes and long time scales, we utilize machine learning force fields, applying both Gaussian approximation potential and equivariant graph neural networks. We then compare the accuracy of these force fields and discuss the results in regard to the memristive properties of MoS_2. Our findings indicate a reduction in energy barriers for sulfur vacancy diffusion as the size of vacancy clusters increases and highlight the importance of certain interstitial sites in these vacancy clusters.

[1] Li, D., et al. (2018). ACS Nano, 12(9), 9240-9252. doi.org/10.1021/acsnano.8b03977

[2] Spetzler, B., et al. (2024). Adv. Electron. Mater., 10, 2300635. doi.org/10.1002/aelm.202300635

HL 50.9 Thu 17:00 H6

Machine-Learning the Electronic Structure of Twisted Bilayer Graphene — •Lenz Fiedler[1], Agnieszka Kuc[1], Florian Arnold[2], and Attila Cangi[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Dresden, Deutschland — [2]Technische Universität Dresden, Dresden, Deutschland

Twistronics, i.e., the study of twodimensional materials in which individual layers are twisted w.r.t.õne another, has the potential to significantly propel technological progress. Twisted bilayer materials, e.g., graphene, may exhibit a significant change in electronic structure and electrical properties based on twist angle. Their computational treatment with density functional theory (DFT) proves difficult, as small twist angles affect the periodicity of the cell and can only be simulated with large unit cells. In this talk, the recently introduced Materials Learning Algorithms (MALA) - a framework for accelerating DFT calculations based on machine learning - is applied to twisted bilayer graphene. Bilayer graphene serves as a proxy for the larger field of twistronics itself. It is shown how the electronic structure, including electronic density of states and electronic charge density, can be predicted from a small number of twist angles for a range of twisted bilayer graphene structures. Since the MALA framework uses the local density of states to encode the electronic structure on a numerical grid, predictions can be made on much larger length scales than with standard DFT calculations. This work demonstrates how machine learning can be used to computationally model twisted bilayer structures where standard first-principles methods are not viable.

HL 50.10 Thu 17:15 H6

High-throughput *ab initio* screening of 2D heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], Roman Kempt[1], and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Heterostructure interfaces produced by stacking two-dimensional (2D) materials facilitate the development of advanced electronic functionalities down to the atomic level. The efficient autonomous creation and computational study of these systems is, however, a challenge due to the general incommensurability of the 2D monolayers. This often results in large unit cells with hundreds to thousands of atoms.

Here, we present an extensive *ab initio* screening of heterostructures made of 2D systems. The approach makes use of the AFLOW-Hetbuilder – a newly developed tool that automates the heterotructure generation based on coincidence lattice theory [1,2]. It is fully integrated into the AFLOW framework [3,4]. We study the binding energy of a large set of heterostructures and also analyse their structural, electronic, and magnetic properties [5]. The presented efficient workflow can enable the systematic data-driven design of 2D heterostructures.

[1] D. S. Koda *et al.*, J. Phys. Chem. C **120**, 10895 (2016).
[2] https://zenodo.org/record/4721346.
[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[4] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[5] A. Nihei *et al.*, manuscript in preparation (2024).

HL 50.11 Thu 17:30 H6

Size-Dependent Diffusion of Radioactive Alcohols Through CNMs — •Neita Khayya, Andre Beyer, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Conventional membranes frequently struggle to achieve both, high permeance and high selectivity. On the other hand, two-dimensional membranes demonstrated remarkable progress. For example, nanometer-thin carbon nanomembranes (CNMs) from self-assembled monolayers of terphenylthiol molecules combine rapid water permeation with a rejection of ethanol in pressure-driven experiments as well as ultrahigh ionic exclusion in ion conductivity measurements. Although there has been great progress in understanding the distinctive characteristics of CNMs, more work is required to fully understand their transport characteristics, which requires complementary approaches. In this work, we employed the radio-active tracer diffusion method to study the size-depended concentration-driven permeation of different alcohols, namely [14C] CnH2n+1OH (n = 1*3) through thickness-varied CNMs from biphenylthiol (BPT), terphenylthiol (TPT) as well as quaterphenylthiol (QPT) molecules. Our findings align with vaporous alcohol pressure-driven permeation measurements regarding the size exclusion through CNMs. Interestingly, our results indicate an increased permeation rate in the liquid phase, which can be rationalized by hydrogen bonds created inside the membrane between the water molecules and diffused alcohols.

HL 51: Transport Properties (joint session HL/TT)

Time: Thursday 15:00–17:15 Location: H13

HL 51.1 Thu 15:00 H13

Quasi-Ballistic Transport in Phase-Pure GaAs/InAs Core/Shell Nanowires — •Farah Basarić[1,2], Vladan Brajović[1,2], Gerrit Behner[1,2], Kristof Moors[1], William Schaarman[1], Raghavendra Juluri[3], Ana M. Sanchez[3], Hans Lüth[1,2], Detlev Grützmacher[1,2], Alexander Pawlis[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Core/shell GaAs/InAs nanowires represent tubular conductors due to their insulating core and confined conducting states in the InAs shell. We investigate nanowires with a crystalline phase purity of the InAs shell, where reduced scattering in electronic transport is expected. Low-temperature gate-dependent transport measurements give us insight into different contributions to the oscillatory behavior in the magnetoconductance, as well as the possibility to probe non-local transport phenomena due to large phase coherence length. With temperature-dependent measurements, we resolved the quasi-ballistic transport regime, and estimate the phase coherence length. Both measurements indicate superior transport properties of phase-pure GaAs/InAs nanowires in contrast to previous reports on non-phase pure nanowires. Our findings are an important optimization step for further development of nanowire-based hybrid devices.

HL 51.2 Thu 15:15 H13

Influence of defects and shape of thin InAs nanowires on their thermal conductivity, assessed via machine-learning potentials — •Sandro Wieser[1], YuJie Cen[1], Georg K. H. Madsen[1], and Jesús Carrete[2] — [1]Institute of Materials Chemistry, TU Wien, Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Nanowires (NWs) grown from the zincblende (ZB) phase of InAs in the (111) direction commonly contain twin boundary defects consisting of narrow wurtzite (WZ) (001) phase regions between ZB sections. To investigate the impact of these and other defects on heat transport, we employ Green-Kubo equilibrium molecular dynamics simulations utilizing cepstral analysis to efficiently process the noise, and an accurate MACE model trained via active learning strategies to achieve transferability for a wide range of surface conditions.

We show that these twin boundaries reduce the thermal conductivity with respect to that of defect-free WZ-phase (001) NWs by a factor of more than two and that surface conditions lead to lower thermal conductivity values for defect-free ultrathin InAs ZB NWs. Analysis of the shape of twinning NWs reveals that structures mimicking experimentally measured surface configurations can enhance heat transport compared to strictly hexagonal NWs. Additional insights are gained from an analysis of line-group symmetries and vibrational properties for various NW shapes. Furthermore, experimentally motivated symmetric and symmetry-breaking surface defects are studied to reveal more and less influential defect sites.

HL 51.3 Thu 15:30 H13

Ab-initio heat transport in defect-laden quasi-1D systems from a symmetry-adapted perspective — •Yujie Cen[1], Sandro Wieser[1], Georg Kent Hellerup Madsen[1], and Jesús Carrete Montaña[2] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Due to their aspect ratio and wide range of thermal conductivities, nanotubes hold significant promise as heat-management nanocomponents. However, one major limitation preventing their widespread use is the typically high thermal resistance that arises from defects or contact with other materials. An intriguing question is the role that structural symmetry plays in thermal transport through those defect-laden sections. However, the ab-initio study of lattice thermal transport is hindered by factors such as the large number of atoms involved and the artifacts introduced by formalism designed for 3D systems.

We employ an Allegro-based machine learning potential to calculate the force constants and phonons of single and multi-layer MoS_2-WS_2 nanotube with near-DFT accuracy and efficient scaling. Subsequently, we combine representation theory with the mode-resolved Green's function method to calculate detailed phonon transmission profiles across defects, and connect the transmission probability of each mode to structural symmetry. while more drastic symmetry breakdowns might be expected to increase scattering and thermal resistance, our results show they actually reduce it by the suppression of selection rules and opening more phonon transmission channels.

HL 51.4 Thu 15:45 H13

Analysis of the electrical transport properties of MBE grown cubic Galliumnitride (c-GaN) sample structures — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor system for 'more-than-Moore' applications such as high-power electronics or optoelectronic devices. The analysis of its electrical transport properties is challenging since the molecular beam epitaxy (MBE) growth of high-quality c-GaN thin films requires a complex substrate architecture in order to accommodate the lattice mismatch between c-GaN and the 3C-SiC template. However, a reliable characterization of the electrical transport properties of c-GaN is crucial for the design of advanced functional devices. Here we analyze the electrical transport properties of the whole sample structure (MBE grown c-GaN/c-AlN thin films onto a 3C-SiC/Si template) with different c-GaN thicknessses using electrochemical impedance spectroscopy (EIS) as well as angle- and temperature-dependent magnetoresistance (MR) measurements. MR measurements reveal the existence of a highly conductive channel while EIS measurements allow the determination of the position of the channel between the c-AlN thin film and the 3C-SiC layer.

15 min. break

HL 51.5 Thu 16:15 H13

Fabrication and Characterisation of Short-channel Junctionless Nanowire Transistors — •Alessandro Puddu — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The downscaling limitations of conventional planar transistors require the investigation of alternative device configurations. Because of their excellent electrostatic control and intrinsic scalability, junctionless nanowire transistors (JNTs) present a feasible solution and are highly desirable for next-generation electronics. The key factor that characterizes the JNTs is the absence of pn-junctions. This provides several benefits, such as an easier fabrication process since the devices do not require abrupt doping profiles within the nanowire channel, which is now uniformly doped.

This work focuses on the fabrication and characterisation of short-channel Si JNTs. A top-down approach based on e-beam lithography (EBL) and inductively coupled plasma reactive ion etching (ICP-RIE) was used to fabricate the Si nanowires. The device characterisation showed improved performances due to the channel length shrinking.

HL 51.6 Thu 16:30 H13

***Ab initio* investigation of drag effect in germanium** — •Dwaipayan Paul and Nakib Protik — Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany

In a system of interacting electrons and phonons, the transport of one induces transport in the other. This phenomenon is known as the electron-phonon drag effect [1]. Now, an important milestone in the history of drag physics is the first recorded measurement of this phenomenon in germanium [2]. Here we present the results of our *ab initio* computations of the thermoelectric transport coefficients of germanium for various temperatures and charge carrier concentrations using the `elphbolt` code [3]. We investigate how the various scattering channels in the system enable this material to exhibit strong drag phenomena.

[1] Gurevich, Yu G., and O. L. Mashkevich. "The electron-phonon

drag and transport phenomena in semiconductors." Physics Reports 181.6 (1989): 327-394.

[2] Frederikse, H. P. R. "Thermoelectric power of germanium below room temperature." Physical Review 92.2 (1953): 248.

[3] Protik, Nakib H., et al. "The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations." npj Computational Materials 8.1 (2022): 28.

HL 51.7 Thu 16:45 H13

Anomalous Knudsen effect signaling long-lived modes in 2D electron gases — •Grigorii Starkov and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

Careful analysis of electron collisions in two spatial dimensions leads to the conclusion, that the odd harmonics of the electron distribution function decay much slower in comparison to the even ones at finite temperatures. Focusing on a channel geometry with boundary scattering, we show, that such behaviour of the odd decay rates leads to a characteristic behaviour of the resistance that we dub anomalous Knudsen effect: increasing temperature leads to decreasing resistance, that quickly slows down and turns into growth. The further increase of temperature exhibits the usual Gurzhi peak in the resistance related to the crossover from ballistic to hydrodynamic transport. The simultaneous observation of the Gurzhi peak preceded by an anomalous Knudsen dip can serve as a concrete signature of the long-lived modes in the 2D electron transport at low temperatures.

HL 51.8 Thu 17:00 H13

Quantum confinement and stoichiometry fluctuations in nm-thin SiGe layers — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

We simulate biaxially strained SiGe layers of varying thickness in the range of a few nanometers, as found in the base layer of heterojunction bipolar transistors (HBTs). At this length scale, local fluctuations in atomic concentrations can strongly influence the electronic properties of the device, especially the distribution of dopants like e.g. boron. Even at high doping concentrations, only a single atom is present at a 1 nm^2 cross section of the layer on average.

Employing a new parameterization of silicon and germanium in the framework of extended Hückel theory (EHT), we calculate the local band gap for different permutations of the atomic structure. Various distributions of boron atoms are simulated. We study the impact of locally increased and decreased concentrations on the band gap. By varying layer thickness, we evaluate the effects of quantum confinement and how it impacts transport properties of the thin layer in contrast to bulk material.

HL 52: Oxide Semiconductors II

Time: Thursday 15:00–17:15 Location: H14

HL 52.1 Thu 15:00 H14

Connection between electronic structure and crystal symmetry in bismuth vanadate — •Philip Schwinghammer, Franziska Hegner, Frederico Delgado, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The electronic and structural properties of bismuth vanadate (BVO) were characterized using density functional theory (DFT). Previous work in the literature indicated that semi-local exchange was incapable of correctly reproducing the ground-state structure of BVO, but disagreed on which functional would improve the description. We found that the Heyd-Scuseria-Ernzerhof hybrid functional could accurately predict the monoclinic ground state structure, provided spin-orbit coupling was included. Semi-local density functionals mischaracterize the hybridization of the lone pair Bi6s states and O2p states near the valence band edge, which is corrected by hybrid functionals. Due to the large mass of bismuth, spin-orbit coupling is required for an accurate description of the electronic structure. When both corrections are taken into account, we find that the valence and conduction band edges in BVO are extremely flat, leading to large effective masses along one direction in reciprocal space. The effective carrier masses are affected by the ionic structure, indicating a possible reason for the different photo-catalytic efficiencies of tetragonal and monoclinic scheelite BVO.

HL 52.2 Thu 15:15 H14

Blue shift of the absorption onset and bandgap bowing in rutile $Ge_xSn_{1-x}O_2$ — •Elias Kluth[1], Yo Nagashima[2], Shohei Osawa[3], Yasushi Hirose[3], Jürgen Bläsing[1], André Strittmatter[1], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, 113-0033, Japan — [3]Department of Chemistry, Tokyo Metropolitan University, 1-1 Minamiosawa Hachioji, Tokyo 192-0397, Japan

Rutile-GeO_2 has recently attracted increasing research interest as an ultra wide bandgap oxide similar to Ga_2O_3 with the unique advantage that theoretical calculations predict the possibility of ambipolar doping. In contrast rutile-SnO_2 is a well-established transparent conductive oxide (TCO) widely used in solar cells and displays. Alloying SnO_2 with Ge offers a promising pathway to developing deep ultraviolet (DUV) TCOs. However, investigations into the optical properties of the $Ge_xSn_{1-x}O_2$ system remain limited.

In this study, we employed spectroscopic ellipsometry in the visible and ultraviolet region to determine the ordinary dielectric functions of $Ge_xSn_{1-x}O_2$ thin films grown by pulsed laser deposition (PLD) on rutile-TiO_2 substrates. Our analysis reveals a systematic blue shift of the onset of absorption with increasing Ge content. By evaluating the dielectric functions, we extracted the characteristic transition energies at the absorption onset and determined the bowing parameter of the dipole-allowed direct bandgap to be $b = 0.70$ eV.

HL 52.3 Thu 15:30 H14

$NaNbO_3$, $KNbO_3$, and their solid solutions: A *first-principles* and special quasirandom structures investigation — •Daniel Fritsch — Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany — University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

Ferroelectric materials crystallising in the perovskite structure, like $NaNbO_3$ and $KNbO_3$, have come into focus as lead-free and environmentally friendly alternatives to the widely used piezoelectric ceramic $Pb[Zr_xTi_{1-x}]O_3$ (PZT) [1].

They both exhibit a large range of structural phase transitions and accompanying changes in their ferroelectric behaviour. While the material properties of both end members are relatively well known, this is much less the case for their solid solutions.

Here, we present results for $Na_{1-x}K_xNbO_3$ solid solutions based on *first-principles* calculations for the structural and electronic properties, and so-called special quasirandom structures to investigate the solid solutions [2]. The obtained results will be compared to available experimental findings and other theoretical investigations.

[1] D. Fritsch, Adv. Mater. Sci. Eng. **2018**, 6416057 (2018).
[2] D. Fritsch, Appl. Sci. **12**, 2576 (2022), J. Phys. Condens. Matter **36**, 375702 (2024).

HL 52.4 Thu 15:45 H14

Spintronic properties of the two-dimensional electron gas in KTaO3-based heterostructures. — •Sonali Kakkar[1] and Chandan Bera[2] — [1]Department of Physics, Noida Institute of Engineering and Technology, 19, Institutional Area, Knowledge Park II, Greater Noida, Uttar Pradesh 201306, India — [2]Institute of Nano Science and Technology, Sector-81, Knowledge City, Sahibzada Ajit Singh Nagar, Punjab, 140306, India

A two-dimensional electron gas (2DEG) in oxide interfaces offers a single platform for a wide range of functionalities. Compared to STO-based 3d-2DEG, 2DEG in the polar perovskite oxide KTaO3 (KTO) with 5d-t2g orbitals shows a greater atomic spin-orbit coupling. More-

over, the electronic and spintronic properties of oxide heterostructures are greatly influenced by the inherent crystal structure symmetry. In this work, we have investigated the electronic and spintronic properties in KTO-based heterostructures using density functional theory calculations with the Hubbard parameter (DFT+U). The dependence of the Rashba spin-splitting and the corresponding spin texture in the reciprocal space for 2DEG at the KTO surface and LVO/KTO interface on the crystal orientation highlights the importance of crystal symmetry for the 5d-2DEG in KTO [1]. Furthermore, highly confined, spin-polarized 2DEG at the interfacial TaO2 layer in the 5dxy orbitals of Ta at the interface between the ferromagnetic insulator EuO and the non-magnetic KTO shows Rashba spin texture [2]. [1] S. Kakkar, et al., Physica E Low Dimens. Syst. Nanostruct. 144, 115394 (2022). [2] S. Kakkar, et al., Adv. Phys. Res. 2, 2200026 (2023).

15 min. break

HL 52.5 Thu 16:15 H14

Unraveling the mechanism of resistive switching in titanate-based perovskites — Wahib Aggoune[1,2], •Parrydeep Kaur Sachdeva[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany — [2]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Memristors capable of switching between high and low resistance states while retaining memory, hold promise for non-volatile memory. A recent fascinating experimental work observed high resistive switching (RS) in *off*-stoichiometric paraelectric titanate-based perovskites $ATiO_3$ (A=Sr, Ca) [1]. It suggests that RS is driven by defects, though their exact role remains unclear. Here, we investigate the defects behavior using density functional theory. Under the experimental growth conditions, the complex defect (Ti-interstitial with *A*-vacancies) is thermodynamically stable, pinning the Fermi level close the conduction band. Remarkably, the *off*-center shift of the interstitial atom induces a local polarization and gives rise to localized mid-gap states. Switching between the equivalent *off*-center sites faces energy barriers of 0.1–0.8 eV, depending on the pathway. This switches both polarization direction and the defect charge distribution. Therefore, upon applying a voltage, the overall polarization driven by the local shifts of the defects can be switched. As this also redistributes the defect charge states, it switches the resistance state. Our findings provide insights into the origin of RS toward memristor development.
[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 52.6 Thu 16:30 H14

Ultraviolet Emission from $^6P_{7/2}$ Stark Manifold in Gd-Implanted β-Ga_2O_3 Thin Films — •Martin S. Williams[1,2], Mahmoud Elhajhasan[1], Marco Schowalter[1], Lewis Penman[3], Alexander Karg[1], Fabien C.-P. Massabuau[3], Andreas Rosenauer[1], Gordon Callsen[1], Carsten Ronning[4], Martin Eickhoff[1,2], and Manuel Alonso-Orts[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany — [3]Department of Physics, SUPA, University of Strathclyde, Glasgow, United Kingdom — [4]Institute of Solid State Physics, Friedrich-Schiller-University Jena, Helmholtzweg 3, 07743 Jena, Germany

Monoclinic gallium oxide (β-Ga_2O_3) is a promising ultra-wide band gap semiconductor for the next generation of optoelectronic devices. Despite its attractive material properties, its luminescence spectrum is dominated by defect emission in the visible spectral range and a dominating UV emission in β-Ga_2O_3 has rarely been observed. An enhancement of the UV emission in β-Ga_2O_3 by optically active ion doping in β-Ga_2O_3 is only achieved with gadolinium (Gd^{3+}).

In this work, β-Ga_2O_3 thin films grown by molecular beam epitaxy and atomic layer deposition are implanted with Gd and thermally activated. Four separate luminescence peaks, from the Stark-split $^6P_{7/2} \rightarrow {}^8S_{7/2}$ transition in Gd^{3+}, are individually resolved with linewidth $\leq$ 2 meV. The influence of growth technique, implantation parameters and annealing temperature is investigated.

HL 52.7 Thu 16:45 H14

Investigation of the bond length dependence and lattice relaxation in zincblende Cu(Br,I) alloys — •Sandra Montag[1], Stefan Merker[2], Michael Bar[1], Richard J. Schenk[1], Eva Zollner[1], Konrad Ritter[1], Timo Pfeiffelmann[1], Sergiu Levcenko[1], Edmund Welter[3], Holger von Wenckstern[1], Marius Grundmann[1], Harald Krautscheid[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

CuI is a promising p-type wide-bandgap semiconductor with various applications in the field of transparent electronics. Among the numerous doping and alloying candidates, the Cu(Br,I) alloy system offers the opportunity to tailor the free hole concentration in functional layers, enabling optimized performance of active devices, such as pn-diodes and transistors. Using X-ray absorption spectroscopy, the fine structure of $CuBr_{1-x}I_x$ powder and thin film samples, with anion composition x varying from 0 to 1, was measured. The analysis of the extended fine structure reveals a nonlinear change of the Cu-Br and Cu-I bond lengths with composition x. This behaviour is different from that reported for III-V and II-VI zincblende alloys, but comparable to the rocksalt $RbBr_{1-x}I_x$ alloy. The observed bond length bowing may therefore be a characteristic feature of group I-VII alloys. To uncover the degree of lattice relaxation with increasing distance from the absorbing atom, the higher neigbour scattering signal is evaluated.

HL 52.8 Thu 17:00 H14

Revealing the incorporation site and local structure of Ni and Se in doped CuI thin films — •Mustafa G. Yazlak[1], Christiane Dethloff[1], Philipp Storm[1], Michael Lorenz[1], Sandra Montag[1], Hans H. Falk[1], Edmund Welter[2], Sofie Vogt[1], Marius Grundmann[1], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

This study investigates polycrystalline CuI thin films with varying nickel (Ni) and selenium (Se) concentrations, grown on glass substrates using Pulsed Laser Deposition (PLD) and co-sputtering. CuI:Ni thin films, with 1*30 at% Ni and thicknesses between 0.1*1.0 μm, and CuI:Se thin films, with 0.4*3.8 at% Se and $\sim$1.0 μm thickness, were prepared and capped with Al_2O_3 layers to prevent oxidation. X-ray Absorption Spectroscopy (XAS) at low temperatures ($\sim$10 K) was conducted at the Cu, Se, and Ni K-edges to study the local structure of Ni and Se in the CuI matrix. The near edge structure and extended fine structure for a pure CuI thin film at the Cu K-edge suggests possible Cu oxidation. For CuI:Ni thin films, an increase in Ni concentration correlates with reduced Cu oxidation because Ni prefers to bond with oxygen rather than iodine, forming disordered NiO as seen from the Ni K-edge spectra. For CuI:Se thin films, the Cu K-edge spectra show small changes but no clear trend with Se content and the Se K-edge spectra indicate a Cu neighborhood similar to Cu_2Se and CuSe. Quantitative analyses are in progress to provide a deeper understanding of how Ni and Se content affects local structural changes.

HL 53: 2D Semiconductors and van der Waals Heterostructures V

The session covers excitonic properties of 2D semiconductors and van der Waals heterostructures.

Time: Thursday 15:00–17:15 Location: H15

HL 53.1 Thu 15:00 H15

1D exciton confinement in monolayer $MoSe_2$ near ferroelectric domain walls in periodically poled $LiNBo_3$ — •Pedro Soubelet, Yao Tong, Asier Astaburuaga Hernandez, Andreas V. Stier, and Jonathan J. Finley — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Monolayer transition metal dichalcogenides are an emergent platform for exploring and engineering quantum phenomena in condensed matter. Due to their atomic thickness, the excitonic response is highly influenced by the dielectric environment. In this work, we explore the optical properties and exciton kinetics of monolayer thick $MoSe_2$ straddling domain wall boundaries in ferroelectric periodically poled $LiNbO_3$ (PPLN). Spatially resolved photoluminescence (PL) experiments reveal sorting of neutral and charged excitons across the boundary. Our results reveal evidence for extremely large in-plane electric fields ($\simeq$4000 kV/cm) at the domain wall (DW), whose effect is manifested in the routing of free charges and trions towards oppositely poled domains, resulting in a nonintuitive spatial PL intensity pattern. In a second step, we engineer the PPLN substrate and the 2D heterostructure to exploit the non-uniform in-plane electric field exerted by the DW to confine neutral excitons in a 1D dipolar gas. Reducing the dimensionality holds an excellent potential for unlocking strong exciton-exciton interaction regimes, enabling exploration of exotic quantum phases of matter and designing advanced optoelectronic devices.

HL 53.2 Thu 15:15 H15

Collective charge excitations between moiré minibands in twisted WSe_2 bilayers probed with resonant inelastic light scattering — •Hendrik Lambers[1], Nihit Saigal[1,2], Nicolai-Leonid Bathen[1], Veljko Antić[1], Lennart Klebl[3], Dante M. Kennes[4], Tim O. Wehling[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]EMBL Imaging Centre, Heidelberg, Germany — [3]Institute of Theoretical Physics, University of Hamburg, Germany — [4]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany

The weak van der Waals coupling between monolayers of transition-metal dichalcogenides (TMDCs) allows the realization of twisted van der Waals structures resulting in precisely tailored 2D quantum systems with superimposed moiré superlattice structures. These are dependent on twist angle and lattice constant mismatch and can cause flat moiré mini bands in the reduced Brillouin zone of the superlattice. Here we study these moiré minibands in $tWSe_2$ homobilayers encapsulated in hBN by low temperature resonant inelastic light scattering (RILS) [1]. Guided by theoretical predications, we identify single particle-like collective inter moiré miniband excitations. Thereby, we establish RILS as a tool to quantitatively probe the formation of moiré minibands. Furthermore, we identify local twist angle variations by lateral force microscopy and correlate these findings with optical (Raman) spectroscopy. [1] N. Saigal et al., Phys. Rev. Lett. 133, 046902 (2024).

HL 53.3 Thu 15:30 H15

Unraveling Rashba spin-orbit coupling in TMDs — •Miguel Morales Cocera[1,2], Marta Prada[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Transition metal dichalcogenides (TMDs) possess unique optical and electronic properties, making them ideal candidates for exploring new physical phenomena. Their significant spin-orbit coupling enables a rich landscape of spin-valley physics within the realm of excitonic effects or topologically non-trivial materials, to name a few. However, there are still unanswered questions concerning the mechanisms that rule Rashba spin-orbit coupling (RSOC), such as the role of the atomic and orbital composition, number of layers, or band character. In this work, we employ ab-initio calculations together with perturbative approaches to unravel the intricacies of bilayer TMDs with an intrinsic dipole, which is far from trivial. We deliver with high numerical precision the Rashba parameters in Rmx (Bernal stacking) bilayers (M= Mo, W. X=S, Se, Te).

HL 53.4 Thu 15:45 H15

Theory of Magnetic Field Dependence of Excitonic Spectra in Atomically Thin Semiconductors — •Michiel Snoeken and Henry Mittenzwey — Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany

The linear absorption spectrum of TMDC monolayers under the influence of an in-plane magnetic field is theoretically studied in an excitonic picture. It is shown that in-plane magnetic fields induce a hybridization between spin-bright and spin-dark exciton transitions, resulting in a brightening of spin-dark excitons in the linear absorption spectrum with increasing in-plane field-strength. Numerical evaluation shows that with increasing field strength, not only the energy splitting between bright and dark excitonic resonances increases, but also an impact on the respective excitonic linewidths can be observed. Some limiting cases are investigated analytically, allowing to discuss a detailed physical picture of the magnetic field-dependent excitonic energies and linewidths.

15 min. break

HL 53.5 Thu 16:15 H15

Spatial mapping of the tunable band gaps of bilayer graphene using a WSe_2 sensor layer — David Tebbe[1], •Alexander Polkowski[1], Sophia Lackhoff[1], Jonas Blum[1], Takashi Taniguchi[2], Kenji Watanabe[2], Bernd Beschoten[1,3], Lutz Waldecker[1], and Christoph Stampfer[1,4] — [1]2nd Institute of Physics A, RWTH Aachen University, Aachen — [2]National Institute for Materials Science, Namiki, Tsukuba, Japan — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [4]Peter Grünberg Institute (PGI-9) Forschungszentrum Jülich, Jülich, Germany

Bernal bilayer graphene (BLG) is a 2D material with promising properties for future quantum technologies, due to its tunable band gap and rich correlated phases, which have been detected by electrical transport measurements. However, due to their nature, these measurements have not been able to spatially resolve the bandgap and other electronic properties of BLG. Here, we show optical sensing can overcome this limitation. To achieve this we place a sensing monolayer of WSe_2 in direct contact to BLG in a double-gated device structure. The sensor layer hosts excitons, with the ability to sense changes in the electronic configuration of the BLG. The WSe_2 hosts Rydberg excitons, which are sensitive to the surrounding dielectric environment and thus sense small changes in carrier density within the BLG, allowing to observe the band gap opening. These excitonic states can be resolved using white light reflection spectroscopy, which allowed us to spatially map the potential landscape in the BLG.

HL 53.6 Thu 16:30 H15

Beyond the K-Valley: Exploring Unique Trion States in Indirect Band Gap Monolayer WSe_2 — •Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Atomically thin layers of transition metal dichalcogenides are of great interest due to their exceptional electronic and optical properties. Their lack of inversion symmetry and strong spin-orbit interaction from heavy metal atoms leads to an additional valley degree of freedom and significant spin splittings in the Brillouin zone. The reduced dimensionality and dielectric screening make these materials ideal for studying Coulomb-bound many-body states, such as excitons and trions.

We will discuss calculations of the optical properties of monolayer WSe_2 using *ab initio* many-body screened configuration interaction. We'll highlight our findings on additional species of negatively charged trions including the **Q**-valley, which we found to be more energetically favorable than those in the **K**-valley. Our results align well with ex-

perimental data and provide new insights into previously observed but unexplained optical features. Furthermore, we will analyze the many-body interactions that reveal the mechanisms behind the increased singlet-triplet splitting and the redshifted energies in the **Q**-valley trions compared to those in the **K**-valley.

HL 53.7 Thu 16:45 H15

Trion saturation and trion filtering in MoS_2 and MoS_2/graphene heterostructures — Omid Ghaebi[1], Tarlan Hamzayev[1], •Till Weickhardt[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Abbe Center of Photonics, Friedrich Schiller University Jena

Optical excitation of electron-hole pairs in transition-metal dichalcogenides leads to the formation of excitons, that can join with free carriers to form trions [1]. Since trions display an efficient non-radiative decay, tuning their relative density with respect to neutral excitons by external knobs is fundamental to engineer the light emitting efficiency of TMD opto-electronic devices. In this work, we investigate the interplay of excitons, trions, and free electrons with regards to gating and excitation power. By carrying out these experiments on a pristine MoS_2 monolayer as well as on a MoS_2/graphene heterostructure where the graphene facilitates fast charge transfer from the TMD [2,3], we study the interdependent dynamic of excitons and trions. Most prominently, this effect can be seen in a super-linear power-scaling of the exciton density due to saturation of trions in the monolayer MoS_2 [4]. When the graphene is added to form the heterostructure, this effect vanishes due to the elimination of trions.

[1] Mak et al. Nature Mater 12, 207-211 (2013). [2] Lorchat et al. Nat. Nanotechnol. 15, 283-288 (2020). [3] Küchle et al. Opt. Mater.: X 12, 2590-1478 (2021). [4] Wang et al. ACS Photonics 10 (2), 412-420 (2023).

HL 53.8 Thu 17:00 H15

Engineering carrier density and exciton polarization in WSe2 monolayers via photochlorination — •Eirini Katsipoulaki[1,2], George Vailakis[1,3], Delphine Lagarde[4], Vishwas Jindal[4], Konstantinos Mourtzidis[4], Xavier Marie[4], Ioannis Paradisanos[1], George Kopidakis[1,3], George Kioseoglou[1,3], and Emmanouel Stratakis[1,2] — [1]FORTH/IESL, Heraklion, Greece — [2]Dpt. of Physics, UoC, Heraklion, Greece — [3]Dpt. of Materials Science and Engineering, UoC, Heraklion, Greece — [4]Universite de Toulouze, INSA-CNRS-UPS, LPCNO, Toulouze, France

Transition Metal Dichalcogenides (TMDs) represent a special class of 2D van der Waals materials. Unlike their 3D-counterparts, which are indirect gap semiconductors, the monolayers exhibit a direct bandgap, leading to a significant enhancement in photoluminescence quantum yield. TMDs feature valley dependent optical selection rules, establishing them as promising candidates for atomically thin optoelectronic devices. A key factor influencing the performance of TMDs in these applications is the carrier density. To address this, we demonstrate the modulation of the Fermi level in WSe2 monolayers using an UV-assisted photochlorination method. Systematic shifts and relative intensities between charged and neutral excitons indicate a controllable decrease of the electron density and switch WSe2 from n- to a p-type semiconductor. DFT calculations predict Cl2 adsorption at Se vacancies. Furthermore, this method can strongly impact the circular polarization degree of excitons. These findings indicate that photochlorination can tailor nanopatterned lateral p-n junctions.

HL 54: Ultra-fast Phenomena II

Time: Thursday 15:00–17:15 Location: H17

HL 54.1 Thu 15:00 H17

Effect of the acceptor strength on intermolecular conical intersection dynamics in aggregates of quadrupolar dyes — •Katrin Winte[1], Somayeh Souri[1], Daniel Lünemann[1], Teresa Kraus[2], Elena Mena-Osteritz[2], Peter Bäuerle[2], Sergei Tretiak[3], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Ulm University, Germany — [3]Los Alamos National Laboratory, USA

Aggregated films of quadrupolar acceptor-donor-acceptor (A-D-A) molecules have emerged as promising materials for organic photovoltaics. The optoelectronic properties in the molecule are governed by an interplay between electronic and vibronic couplings in the molecule. In aggregated films, we have uncovered the existence of intermolecular conical intersections (CoIn) occurring on timescales of less than 50 fs, which funnel energy from the photoexcited bright state into the lower-lying dark electronic state of the aggregate [1]. This raises the question whether the quantum dynamics of the aggregates can be altered by modifying the intramolecular charge transfer character of the A-D-A monomers. Chemical intuition suggests that increasing the acceptor strength might accelerate charge transfer and with it the passage through the CoIn. To explore this hypothesis, we synthesize thin films of A-D-A molecules with varying acceptor strengths and study their ultrafast dynamics by femtosecond time-resolved spectroscopy. Our results show only minimal effects on the CoIn dynamics, suggesting that intermolecular vibronic couplings play the dominant role in the quantum dynamics. [1] A. De Sio et al., Nature Nano 16, 63 (2021).

HL 54.2 Thu 15:15 H17

Ultrafast decay of spin-polarization of semiconductor holes measured by attosecond transient absorption spectroscopy — •Lauren Drescher[1,2], Kylie Gannan[1], and Stephen Leone[1] — [1]Department of Chemistry, University of California, Berkeley, California 94720, USA — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

Carrier excitation by light can lead to spin-polarization in semiconductor conduction and valence bands. While the dynamics of the spin-polarization of conduction band electrons are often well characterized, comparably little is known about the counterpart polarization of valence band holes, due to its much shorter lifetime.

Here we introduce circular dichroic attosecond transient absorption spectroscopy which allows to follow the spin-polarization of materials on attosecond timescales through coupling to the angular momentum of light. Corroborated by real-time time-dependent density functional theory calculations, our experimental results reveal the few femtosecond decay of semiconductor hole spin-polarization in germanium. Our method opens the door to measure spin dynamics in non-magnetic materials with extreme temporal resolution, high spectral resolution and core-level specificity.

HL 54.3 Thu 15:30 H17

Picosecond Femtojoule Resistive Switching in Nanoscale VO2 Memristors — •Sebastian Schmid[1,2], Laszlo Posa[1,3], Timea Török[1,3], Botond Santa[1,4], Zsigmond Pollner[1], György Molnar[3], Yannik Horst[5], Janos Volk[3], Juerg Leuthold[5], Andras Halbritter[1,4], and Miklos Csontos[5] — [1]Department of Physics, Institute of Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86159, Germany — [3]Institute of Technical Physics and Materials Science, HUN-REN Centre for Energy Research, 1121 Budapest, Hungary — [4]HUN-REN-BME Condensed Matter Research Group, H-1111 Budapest, Hungary — [5]Institute of Electromagnetic Fields, ETH Zurich, 8092 Zurich, Switzerland

The dynamics of the Mott transition in correlated electron oxides could provide a sustainable alternative to the von Neumann computation by exploiting device-level functional complexity at low energy consumption. We fabricated nanoscale VO2 devices and tested them in our picosecond timeresolution, real-time resistive switching experiments, using 20 ps short and <1.7 V amplitude voltage pulses. There we observed tunable resistance states from insulator-metal transitions with down to 15 ps incubation times and switching energies starting from a few femtojoule. These orders of magnitude improvements from other memristive devices open up new possibilities for neuromorphic computing applications, outperforming the human brain at size and speed, with competitive energy consumption.

HL 54.4 Thu 15:45 H17

Agreement between Theoretically Predicted and Measured Bragg Peak Decay in Bismuth Following Femtosecond Laser Excitation — •Bernd Bauerhenne[1], Jimiben Patel[1], Sahar Bakhshi[1], Sascha Epp[2], and Martin Garcia[1] — [1]Institute of

Physics, University of Kassel, Heinrich-Plett-Straße 40, D34132 Kassel, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, 3 Luruper Chaussee 149, 22761 Hamburg, Germany

We investigated the time-resolved Bragg peak decay in bismuth films, 30 nm and 50 nm thick, following excitation with femtosecond (fs) laser pulses. These measurements were conducted using x-ray pulses sourced from a free-electron laser. To explain the observed Bragg peak decay, we developed an electronic temperature (Te) dependent interatomic potential for bismuth, generated using forces and energies from ab initio molecular dynamics (MD) simulations at elevated Te levels. Additionally, we computed the optical properties and the Te-dependent electron-phonon coupling constant for bismuth using ab initio methods. Employing these calculated quantities, we conducted MD simulations on similarly laser-excited antimony films, 30 nm and 50 nm thick. The comparison between our theoretical predictions and experimental measurements of Bragg peak decay exhibited an agreement, affirming the accuracy of our model. This model effectively incorporates the fs-laser induced modifications of the potential energy surface and the dynamic influences of electron-phonon coupling, providing a robust framework for understanding laser-material interactions in ultrafast processes.

15 min. break

HL 54.5 Thu 16:15 H17

Ultrafast Time-Domain Spectroscopy Reveals Coherent Vibronic Couplings Upon Electronic Excitation in Crystalline Organic Thin Films — •Naby Hadilou[1], Somayeh Souri[1], Daniel Timmer[1], Daniel C. Lünemann[1], Katrin Winte[1], Antonietta De Sio[1], Martin Esmann[1], Sebastian Anhäuser[2], Michele Guerrini[1], Ana M. Valencia[1], Caterina Cocchi[1], Gregor Witte[2], and Christoph Lienau[1] — [1]Oldenburg university, Germany — [2]Philipps-Universität Marburg, Germany

Coherent coupling between electronic excitations and molecular vibrations significantly influences the optical and charge transport properties of organic semiconductors and may have profound effect on technologically relevant processes such as excitons fission. Highly ordered crystalline films are ideal for probing such couplings since they enable studies of individual domain. Here, we report first polarization-resolved pump-probe experiments probing the ultrafast dynamics of crystalline perfluoropentacene thin films grown on different substrates with 10-fs time resolution. Coherent oscillations in the spectra reveal vibronic couplings to a high-frequency, 25-fs, in-plane deformation mode that is insensitive to the optical polarization, while the coupling to a lower-frequency, 85-fs, out-of-plane ring bending mode depends significantly on the crystalline and molecular orientation. Raman spectra confirm this interpretation and highlight the dominance of solid-state effects on vibronic couplings. Our results represent a first step toward uncovering the role of anisotropic vibronic couplings for singlet fission processes in crystalline molecular thin films.

HL 54.6 Thu 16:30 H17

Attosecond light-driven charge injection in germanium — •Giacomo Inzani[1,9], Lyudmyla Adamska[2,3], Amir Eskandariasl[4], Nicola Di Palo[1], Gian Luca Dolso[1], Bruno Moio[1], Luciano Jacopo D'Onofrio[4,5], Alessio Lamperti[6], Alessandro Molle[6], Rocio Borrego-Varillas[7], Mauro Nisoli[1,7], Stefano Pittalis[2], Carlo Andrea Rozzi[2], Adolfo Avella[4,5,8], and Matteo Lucchini[1,7] — [1]Dept. of Physics, Politecnico di Milano, Italy — [2]CNR - Istituto Nanoscienze, Modena, Italy — [3]Dept. of Physics, Mathematics and Informatics, University of Modena & Reggio Emilia, Italy — [4]Dip. di Fisica, Università degli Studi di Salerno, Italy — [5]CNR - SPIN, UoS di Salerno, Italy — [6]CNR - IMM, Unit of Agrate Brianza, Italy — [7]IFN - CNR, Milano, Italy — [8]Unità CNISM di Salerno, Università degli Studi di Salerno, Italy — [9]Present address: Dept. of Physics, University of Regensburg, Germany

The injection of charges from the valence to the conduction band of a semiconductor induced by an ultrashort pulse can tailor its electro-optical properties. This process typically occurs on time scales shorter than the laser period - for visible light, in the order of one femtosecond. Despite its relevance, few experiments studied the charge excitation process with attosecond temporal resolution. In this work, we combine attosecond transient reflection spectroscopy measurements to a dual cutting-edge theoretical approach, demonstrating that photoexcitation in Ge cannot be ascribed to a single physical mechanism. The interplay of multi-photon absorption, light-induced band dressing, and intra-band motion is crucial for determining the overall charge injection.

HL 54.7 Thu 16:45 H17

Dephasing Effects in High-Harmonic Generation from Solids — •Francisco Navarrete and Dieter Bauer — Institut für Physik, Universität Rostock, 18051 Rostock, Deutschland

In the calculation of high-order harmonic generation (HHG) in solids, introducing a dephasing time is often crucial for accurately reproducing the distinct spectral peaks observed experimentally in the first plateau region [1,2]. In this contribution, we present analytical and numerical studies on the non-integer contributions to the interband HHG spectrum and investigate how dephasing affects not only the spectral structure but also the amplitude and wavelength dependence of the harmonics. Using a simplified two-band model, we numerically solve and also approximate the semiconductor Bloch equations via a saddle-point method [3] to elucidate these effects. Our findings provide closed analytical expressions for these contributions, offering insights into the interplay between dephasing and electron dynamics in solids and the mechanisms shaping the HHG spectrum.

References:
[1] Vampa et al., Phys. Rev. Lett. 113, 073901 (2014)
[2] Cavaletto et al., Nat. Rev. Phys. (2024) (accepted)
[3] Navarrete et al., Phys. Rev. A 100, 033405 (2019)

HL 54.8 Thu 17:00 H17

Ultrafast Dynamics of Vanadium Dioxide Phase Transformation — •Liuyue Yang, Daniel Sandner, and Hristo Igle — Laser and X-Ray Physics E11, TUM School of Natural Sciences, TUM, James-Franck-Str. 1 85748 Garching, Germany

Vanadium dioxide has been discovered to have a metal-to-insulator transformation (MIT) at 68 °C. To investigate the dynamics of MIT, we use the pump-probe experiment to obtain the reflective transient mid-infared spectrum of VO2. In the photoinduced VO2 MIT, the phase transformation can occur at high pump power. The reflectivity of VO2 increases significantly at the metal state. At high temperature, the phase transformation occurs at lower pump power. Moreover, we observed a reflectivity oscillation in wavelength around the zeropoint of pump delay. The oscillation frequency decreases rapidly with the delay time

HL 55: Graphene and 2D Materials (joint session TT/HL)

Time: Thursday 15:00–18:30 Location: H33

HL 55.1 Thu 15:00 H33

Magnetotransport of the Radial Rashba Spin-Orbit Coupling in Proximitized Graphene — •Wun-Hao Kang[1,2], Ming-Hao Liu[1,2], and Denis Kochan[2,3] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

Graphene-based van der Waals heterostructures take advantage of tailoring spin-orbit coupling (SOC) in the graphene layer by the proximity effect. The proximity effect can be effectively modeled by the tight-binding Hamiltonian involving novel SOC terms[1] and allows for an admixture of the tangential and radial spin-textures[2]. Taking such effective models we perform realistic large-scale magnetotransport calculations–transverse magnetic focusing–and show that there are unique qualitative and quantitative features allowing for an unbiased experimental disentanglement of the conventional Rashba SOC from its novel radial counterpart, called here the radial Rashba SOC. Along with that, we propose a scheme for a direct estimation of the Rashba angle by exploring the magneto response symmetries when swapping an in-plane magnetic field[3].

[1] M. Gmitra et al., Phys. Rev. B 93, 155104 (2016).
[2] K. Zollner et al., Phys. Rev. B 108, 235166 (2023).
[3] W.-H. Kang et al., Phys. Rev. Lett. 133, 216201 (2024).

HL 55.2 Thu 15:15 H33

Nonequilibrium Spin Transport in Graphene Proximitized by WSe_2 — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Spin-orbit coupling (SOC) in graphene is known to be negligibly weak, on the order of 0.1 meV, due to its composed atom, carbon, a light element of atomic number only 6. A decade ago, it was found that the SOC in graphene can be significantly enhanced simply by attaching it to a transition metal dichalcogenide of strong SOC, known as the spin-orbit proximity effect. Our recent theoretical work in collaboration with a transport experiment on graphene proximitized by WSe_2 reported a supporting number for the SOC as strong as 12.6 meV [1]. Inspired by this finding, here I present numerical results on nonequilibrium spin Hall accumulation in graphene/WSe_2 heterostructures based on the Landauer-Keldysh formalism [2]. Combined with the recently discussed radial Rashba SOC [3], nonequilibrium spin precession will be shown, paving an alternative way to realize the Datta-Das spin transistor.

[1] Q.Rao *et al.*, Nat. Commun. **14**, 6124 (2023);
[2] B.K.Nikolic *et al.*, Phys. Rev. Lett. **95**, 046601 (2005);
[3] W.-H.Kang,M.Barth,A.Costa,A.Garcia-Ruiz,A.Mrenca-Kolasinska, M.-H.Liu, D.Kochan, Phys. Rev. Lett. **133**, 216201 (2024).

HL 55.3 Thu 15:30 H33

Resistively Detected Electron Spin Resonance and g Factor in Few-Layer Exfoliated MoS_2 Devices — •Chithra H. Sharma[1,2], Appanna Parvangada[2], Lars Tiemann[2], Kai Rossnagel[1,3], Jens Martin[4], and Robert H. Blick[2,5] — [1]Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany — [5]University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA

MoS_2 has recently emerged as a promising material for enabling quantum devices and spintronic applications. In this context, the demonstration of resistively detected electron spin resonance (RD-ESR) and the determination and improved physical understanding of the g factor are of great importance. However, its application and RD-ESR studies have been limited so far by Schotttky or high-resistance contacts to MoS_2. Here, we exploit naturally n-doped few-layer MoS_2 devices with ohmic tin (Sn) contacts that allow the electrical study of spin phenomena. Resonant excitation of electron spins and resistive detection is a possible path to exploit the spin effects in MoS_2 devices. Using RD-ESR, we determine the g factor of few-layer MoS_2 to be $\approx$1.92 and observe that the g factor value is independent of the charge carrier density within the limits of our measurements.

HL 55.4 Thu 15:45 H33

Unifying Recent Experiments on Spin-Valley Locking in TMDC Quantum Dots — Aakash Shandilya[1], Sundeep Kapila[2], Radha Krishnan[3], Bent Weber[3], and •Bhaskaran Muralidharan[2] — [1]Department of Physics, IIT Bombay, Powai, Mumbai-400076, India — [2]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [3]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

The spin-valley qubit promises significantly enhanced spin-valley lifetimes due to strong coupling of the electrons* spin to their momentum (valley) degrees of freedom. Very recently, few experiments on TMDC quantum dots have, for the first time, shared evidence for spin-valley locking at the few-electron limit. Employing quantum transport theory, we numerically simulate the ground- and excited-state transport spectroscopy signatures of these experiments under diverse conditions through a unified theoretical framework, and reveal the operating conditions, based on intrinsic properties, for spin- valley locking. We thus provide a method to experimentally deduce the degree of spin-valley locking based on the SOC strength, inter-valley mixing, and the spin and valley g-factors. Our theoretical analysis provides an important milestone towards the next challenge of experimentally confirming valley-relaxation times using single-shot projective measurements.

[1] A.Shandilya, S.Kapila, R.Krishna, B.Weber B.Muralidharan, ArXiv:2410.21814 (2024).

HL 55.5 Thu 16:00 H33

Estimation of Relaxation Parameters of Spin-Valley Qubits Via Readout Simulations — •Sundeep Kapila, Aparajita Modak, and Bhaskaran Muralidharan — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

Two dimensional (2D)-material quantum dot systems, can host multiple qubit possibilities, namely, spin, valley and the spin-valley qubits. The spin-valley qubit, often referred to as the Kramers qubit, is of special interest due to the possibility of long relaxation and coherence times. Experimentally, such long relaxation times (T_1) have been demonstrated in the bilayer graphene (BLG) platform via Elzerman single-shot readout techniques [1-3]. However, there is a lack of comprehensive synergy in explaining the experimental trends in the relaxation times of different types of qubit possibilities, especially at low magnetic fields [1-3]. Here, we present a detailed master equation-based simulation approach to mimic the Elzerman readout schemes to understand the experimental data presented and to characterize the relaxation processes. Our approach allows us to directly extract from the experimental data, the relaxation rates for individual decay processes. We then extend our analysis to unify various experimental data observed across varying conditions in the BLG platform [1-3]. Our analysis backed up by dedicated machine learning algorithms also enables the extension of the model to qubit systems in the transition metal dichalcogenide platform.

[1] Ennslin et al., Arxiv, Mar 2024
[2] Stampfer et al., Arxiv, Feb 2024
[3] Stampfer et al., Nat. Commun. (2022)

HL 55.6 Thu 16:15 H33

Quantum transport in graphene-based Chern mosaics — •Patrick Wittig[1], Fernando Dominguez[1,2], and Patrik Recher[1,3] — [1]Institute of Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Faculty of Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, 97074 Würzburg, Germany — [3]Laboratory of Emerging Nanometrology, 38106 Braunschweig, Germany

Chern mosaics [1] are systems composed of domains with different Chern numbers within the bulk of the material. Here, the difference in the Chern number between neighboring domains leads to the emergence of chiral boundary modes that propagate along their interface. In our research, we construct a phenomenological scattering network theory based on the symmetries of the system to model the propagation of these chiral modes in triangular and kagome lattice structures, which can arise in graphene-based systems with characteristic valley-chiral edge modes. In particular, we investigate effects such as energy-dependent scattering [2] and spin-orbit coupling [3] within these

networks to analyze the spectrum and transport properties.
[1] S. Grover et al., Nat. Phys. **18**, 885 (2022).
[2] P. Wittig et al., Phys. Rev. B **108**, 085431 (2023).
[3] P. Wittig et al., Phys. Rev. B **109**, 245429 (2024).

HL 55.7 Thu 16:30 H33

Effects of relaxation in deformed graphene structures — Jan Verlage[1], Thomas Stegmann[2], and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, Mexico

It is known that locally deformed graphene creates strong pseudomagnetic fields (of over 100 T) giving rise to Landau levels and being crucial elements of various valleytronic devices. However, taking into account the atomic relaxation of such structures may lead to reduction and regularization of the strain. Here, we revise these effects in various previously studied setups, including membranes and bumps. Our numerical simulations indicate that the atomic relaxation induces a reduction of the pseudomagnetic field by a factor of $5 \div 10$. It may have several consequences for applications.

15 min. break

HL 55.8 Thu 17:00 H33

Landau level mixing in moderately disordered graphene junctions — •Yu-Ting Hsiao and Ming-Hao Liu — Department of Physics,National Cheng Kung University,Tainan 70101,Taiwan

Landau levels are quantized eigenenergy levels in two-dimensional (2D) systems in the presence of an applied perpendicular magnetic field. They are the basic origin of the (integer) quantum Hall effect (QHE). To observe the QHE, i.e., electrical conductance quantized into a sequence of an integer multiple of the universal conductance quantum $\nu * \frac{e^2}{h}$, the sample quality and the strength of the magnetic field typically play the most decisive roles. The cleaner the sample, the weaker the magnetic field required to form the Landau levels. Collaborating with the experiment group led by Prof. Wei Yang from the Institute of Physics(CAS), China, who observed phase shifts of quantized conductance plateaus in ultraclean two-terminal, single-gated graphene devices. From our quantum transport simulations with a systematic tuning of different parameters that could influence the conductance behavior of the graphene device, we found that the experimentally observed phase shift shall arise from the mixing of Landau levels across two neighboring regions with slightly different doping concentrations. Interestingly, we found that the Landau level mixing occurs only when the graphene sample is moderately disordered. In the purely ballistic regime or under strong disorder, the Landau levels mixing fails to form. Our finding reveals a counter-intuitive role played by disorder, possibly also required in other fundamental transport phenomena, such as the Shubnikov-de Haas oscillation.

HL 55.9 Thu 17:15 H33

Dirac meets flat bands: Topological Mottness swap over through hybridization control — Siheon Ryee[1], •Niklas Witt[2,1,3], Lennart Klebl[2,1], Jennifer Cano[4,5], Giorgio Sangiovanni[2], and Tim Wehling[1,3] — [1]Universität Hamburg — [2]JMU Würzburg — [3]Hamburg Centre for Ultrafast Imaging — [4]Stony Brook University — [5]CCQ

Graphene-based multilayer systems provide a versatile platform to explore the interplay between correlation physics and topology. These systems' unique electronic properties arise from their low-energy bands, characterized by significant Berry curvature originating from graphene's Dirac bands, which is believed to play a crucial role in stabilizing emergent correlated states such as superconducting order and various pseudomagnetic states. In this work, we investigate single-site functionalized graphene, where the Dirac bands hybridize with a correlated flat band of localized orbitals. Our findings based on dynamical mean-field theory (DMFT) calculations reveal a hybridization-driven transition between two symmetry-distinct Mott insulators with a protected metallic state emerging in between. Density functional theory (DFT) calculations suggest that the topological transition observed in our model system is achievable in real materials, specifically through the proximity coupling of epitaxial graphene on SiC with group IV intercalants. Unlike phenomena in other correlated graphene-based platforms, such as twisted bilayer graphene and rhombohedral graphene multilayers, the topology-enforced Mottness swap over occurs at a much higher energy scale of electron-volts.

HL 55.10 Thu 17:30 H33

Magnetism in monolayer graphene near 1/4 doping — •Maxime Lucas, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France

Recent studies of twisted bilayer graphene (or other 2D materials) have been stimulated by the discovery of correlations between electronic flat-band states due to a moiré pattern [1]. It is shown experimentally and theoretically that the filling of the flat bands affects their magnetic properties significantly. On the other hand, the effect of doping on a simple graphene layer is still unclear. Indeed, its half-filled case is well known [2], but unlike other lattices [3] its magnetic properties beyond half filling are mostly unexplored, except at 1/4 doping [4]. Here, we present our analysis of graphene magnetism using a combination of the Hubbard model and Hartree-Fock mean-field theory. We work at density values around 1/4 doping (average number of electron per site N_e=0.75) as it puts the system right into one of the Van Hove singularities found in graphene's density of states, giving rise to interesting magnetic properties. We present an interaction-density phase diagram and its associated magnetic orders, described by their band structure and spin structure factor.
[1] Y. Cao et al., Nature 556, 43 (2018); Nature 556, 80 (2018).
[2] M. Raczkowski et al., Phys. Rev. B 101, 125103 (2020), and Refs. therein.
[3] R. Scholle et al., Phys. Rev. B 108, 035139 (2023).
[4] S. Jiang, A. Mesaros, Y. Ran, Phys. Rev. X 4, 031040 (2014).

HL 55.11 Thu 17:45 H33

Electronic transport and anti-super-Klein tunneling in few-layer black phosphorus — •Jorge Alfonso Lizarraga Brito[1], Yonatan Bentancur Ocampo[2], and Thomas Stegmann[1] — [1]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México — [2]Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México, México

The electronic transport of few-layer black phosphorus is analyzed theoretically. This work was performed using recent experimental results obtained by μ-ARPES, where tight-binding parameters up to the 4th nearest neighbors within and between the layers were estimated. It is confirmed that the anisotropic band structure of few-layer black phosphorus leads to highly anisotropic transport properties. Most prominently, it is found that the electrons can pass through a potential barrier aligned in a certain crystallographic direction, while for potential barriers rotated by 90 degrees, the transport is completely blocked (anti-super-Klein tunneling). Finally, the study was extended to the case where the top layer of the system is oxidized, showing that the electronic transport is significantly reduced in the oxidized layers, whereas it can be largely unaffected in the central layers.

HL 55.12 Thu 18:00 H33

Pressure-induced structural phase transitions in the van der Waals multiferroic $CuCrP_2S_6$ — •Swarnamayee Mishra[1] and Jochen Geck[1,2] — [1]Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062 Dresden, Germany

Two-dimensional (2D) crystals with strong in-plane covalent bonds and weak van der Waals (vdW) interlayer interactions have garnered significant attention following the discovery of graphene and its remarkable properties. $CuCrP_2S_6$ (CCPS) is a promising 2D material exhibiting antiferromagnetic behavior due to the collective ordering of Cr^{3+} spins and antiferroelectric properties driven by Cu+ ion ordering. As a type-I multiferroic, CCPS is particularly notable for its coexistence of antiferroelectricity and antiferromagnetism, coupled with strong polarization-magnetization interactions. These ferroic properties arise from spin-orbit coupling associated with crystal symmetry breaking. Despite its potential, a detailed pressure-dependent crystallographic study of CCPS remains unexplored. In this work, we address this gap using high-pressure single-crystal X-ray diffraction (XRD) to investigate the interplay between structural changes and the material's ferroic behaviors. Our study reveals a phase transition from the low-pressure monoclinic Pc phase to the high-pressure monoclinic C2/c phase at low temperatures, providing new insights into the structure-property relationships of this promising 2D vdW material.

HL 55.13 Thu 18:15 H33

^{31}P NMR studies of quasi-two-dimensional (2D) magnetic correlations in $A\mathbf{CrP_2S_6}$ (A = Cu, Ag) — •Saramgi Sivan[1,2], Kizhake Malayil Ranjith[1], Lukas Prager[1,2], Saicha-

ran Aswartham[1], Bernd Büchner[1,2], and Hans-Joachim Grafe[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062

The $AA'P_2S_6$ (A, A' = transition metal ions) family of quasi-2D van der Waals materials has proven to be a model system for low-dimensional magnetism. Here we present detailed ^{31}P NMR measurements on the single crystals of $ACrP_2S_6$. The high-temperature single narrow NMR line shows a splitting at about 160 K for $CuCrP_2S_6$, which is attributed to the antiferroelectric (AFE) transition, while a pake-doublet NMR spectrum is observed for $AgCrP_2S_6$ at room temperature, but no AFE transition at lower temperatures. In $CuCrP_2S_6$, we observed further line splitting below 30 K, reflecting the antiferromagnetic (AFM) order. At $T_N = 30$ K, the NMR spin-lattice relaxation rate $T_1^{-1}(T)$ in $CuCrP_2S_6$ measured at 2.5 T shows a sharp peak due to the critical fluctuations. The T_N is suppressed towards lower temperatures when measured at higher magnetic fields. The $(T_1T)^{-1}(T)$ measured at 7 T shows a broad maximum at about 60 K and a critical enhancement at T_N. On the other hand, $AgCrP_2S_6$ exhibits in-plane AFM order at 20 K, as evidenced by the clear splitting of the NMR spectra, the divergence of $T_1^{-1}(T)$ at T_N, and a broad maximum in the NMR Knight shift. In contrast to $CuCrP_2S_6$, the $(T_1T)^{-1}(T)$ shows only a critical enhancement around T_N without a broad anomaly.

HL 56: Members' Assembly

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2026
- Verschiedenes

Time: Thursday 17:30–19:00 Location: H17

All members of the Semiconductor Physics Division are invited to participate.

HL 57: Quantum Dots and Wires: Optics II

Time: Friday 9:30–13:00 Location: H13

HL 57.1 Fri 9:30 H13

Deterministic Generation of Linear Photonic Cluster States with Semiconductor Quantum Dots: A Detailed Comparison of Different Schemes — •Nikolas Köcher, David Bauch, Nils Heinisch, and Stefan Schumacher — Physics Department, CeOPP, and PhoQS, Paderborn University, Germany

Graph and cluster states are types of multipartite entangled states with applications in quantum communication [1] and measurement-based quantum computation [2]. We theoretically investigate and compare different schemes for the deterministic generation of linear photonic cluster states using spins and trions in charged semiconductor quantum dots under strong Purcell enhancement. The schemes differ in the method used for spin control and whether the emitted photonic qubits are polarization or time-bin encoded. We efficiently track the fidelity and the usable length of the cluster states by calculating the expectation values of their stabilizer generators, assessing their fidelity beyond the calculation of gate fidelities [3]. We find that the performance of the different schemes and which scheme is optimal strongly depend on the cavity environment and the coherence time of the spin qubit.

[1] K. Azuma, K. Tamaki, H.-K. Lo, Nat. Commun. 6, 6785 (2015).
[2] R. Raussendorf, H. Briegel, Phys. Rev. Lett. 86, 5188 (2001).
[3] D. Bauch, N. Köcher, N. Heinisch, S. Schumacher, APL Quantum 1, 036110 (2024).

HL 57.2 Fri 9:45 H13

Scalable integration of site-controlled quantum dots into circular Bragg grating resonators — •Kartik Gaur, Avijit Barua, Sarthak Tripathi, Sam Baraz, Lukas Dworaczek, Neha Nitin, Imad Limame, Aris Koulas-Simos, Priyabrata Mudi, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

The buried-stressor approach [1] is one of the pivotal methods for the growth of site-controlled quantum dots (SCQDs). This growth technique makes use of the strain from a partially oxidized AlAs layer to induce site-selective nucleation of InGaAs quantum dots. Here, we report on growth, fabrication, and surface and optical characterizations of such SCQDs. A systematic investigation of the effects of variation of SCQD growth parameters on QDs density, surface morphology, and optical properties is done using atomic force microscopy (AFM), cathodoluminescence (CL), and microphotoluminescence (μPL) spectroscopy. Moreover, these SCQDs are integrated into circular Bragg gratings (CBGs) in a scalable manner highlighting the advantage of our advanced growth approach. Quantum optical characterizations are also performed on these SCQD-CBGs. The comprehensive understanding of the intricacies involved in the growth and characterization of SCQDs and their scalability in device integration offers a roadmap for the advancement of nanophotonic technologies and quantum information.

[1] A. Strittmatter, et. al., Applied Physics Letters, 100(9):093111, 03 2012.

HL 57.3 Fri 10:00 H13

Spectral correlations of dynamical resonance fluorescence — •Santiago Bermúdez Feijóo[1], Eduardo Zubizarreta Casalengua[2], Kai Müller[2], and Klaus D. Jöns[1] — [1]PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany — [2]Walter Schottky Institute, School of Computation, Information and Technology and MCQST, Technische Universität München, Garching, Germany

In this work, we explore the time-dependent, frequency-filtered [1] photon statistics of a two-level system under pulsed excitation, whose dynamical emission spectrum [2] has been recently experimentally measured using semiconductor QDs [3]. Our results show that photon statistics are not fixed [4] but vary between bunching and antibunching, depending on the applied frequency filters. This reveals an intricate interplay between pulse area, photon frequencies, and correlations, extending insights from the CW case [5]. Notably, frequency-filtering enhances time-bin applications: for odd pulses, it suppresses two-photon events by up to two orders of magnitude, while for even pulses, it restores single-photon purity. This approach simplifies entanglement generation by enabling photon-number control [6] via frequency selection, eliminating the need for complex excitation schemes. [1] E. del Valle et al. PRL 109(18):183601 (2012). [2] Moelbjerg, A. et al. PRL.108, 017401 (2012). [3] Boos, K. et al. PRL.132, 053602 (2024). [4] Fischer, K. et al. Nature Phys 13, 649*654 (2017). [5] J.C. Lopez Carreno et al. Laser & Photonics Reviews, 11(5):1700090 (2019). [6] Wein, S.C et al. Nat. Photon. 16, 374*379 (2022).

HL 57.4 Fri 10:15 H13

Resonance fluorescence measurements on rapid thermally annealed self-assembled quantum dots — H. Mannel[1], •F. Rimek[1], M. Zöllner[1], N. Schwarz[1], N. Bart[2], A. Ludwig[2], A. D. Wieck[2], A. Lorke[1], and and M. Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A single self-assembled quantum dots (QD) is one of the promising candidate as a bright (high photon rate) and stable (fourier-limited) linewidth single photon source [1]. They are typically grown by molec-

ular beam epitaxy (MBE) and have photon emission energies in the near-infrared spectrum. There are several techniques to control the size, which shift the emission wavelength. The so-called indium flush is often used, where the tip of the dot is thermally flushed away [2]. Alternatively, the confinement can be altered by rapid thermal annealing (RTA) [3], which lets indium and gallium diffuse. Here, we investigate the optical properties of rapidly thermally annealed quantum dots. In particular, we study the effects of RTA on the resonance fluorescence line width. This is done by three different measurements. First, we scan over the applied gate voltage and calculate the linewidth using the Stark shift of the exciton. Second, we scan the linewidth directly with a tunable laser. In addition, we study the lifetime in pulsed resonant measurements. The change in the confinement potential might also change dephasing processes such as photoemission or the Auger effect. [1] N. Tomm et al., Nat. N. **16**, 399-403 (2021). [2] H. Sasakura et al., JAP **102**, 013515 (2007). [3] N. Perret et al., PRB **62**, 5092 (2000).

HL 57.5 Fri 10:30 H13

Exploring the limits of absolute position accuracy in single emitter localization microscopy — •Maximilian Heller, Chenxi Ma, Timon Handrup, Yiteng Zhang, Xian Zheng, Micheal Zopf, and Fei Ding — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover

Solid-state single photon emitters (SPEs) integrated in photonic nanostructures provide highly efficient light-matter interfaces for quantum information applications. Wide-field optical positioning has shown the potential to be an inexpensive method with high troughput to achieve the desired spatial matching of SPEs to the nanostructure. However, the accuracy of optical positioning setups has been overlooked so far and mainly the fitting uncertainty has been used as figure of merit. Here, we use arrays of gold nanodisks with pre-defined positions to systematically quantify the main sources of error in fabrication and imaging. From this, we develop a comprehensive calibration model to render the systematic errors insignificant compared to the uncertainties. We demonstrate that the careful calibration of the optical positioning process leads to an increased yield of quantum photonic devices by fabricating and characterizing a large number of circular Bragg gratings around epitaxial quantum dots.

HL 57.6 Fri 10:45 H13

On-demand storage and retrieval of single photons from a semiconductor quantum dot in a room-temperature atomic vapor memory — •Avijit Barua[1], Benjamin Maass[1,2], Norman Vincenz Ewald[1,2], Elizabeth Robertson[2], Kartik Gaur[1], Suk In Park[3], Sven Rodt[1], Jin-Dong Song[3], Stephan Reitzenstein[1], and Janik Wolters[2] — [1]Technische Universität Berlin (TUB), Berlin, Germany — [2]German Aerospace Center (DLR), Berlin, Germany — [3]Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea

Interfacing light from solid-state single-photon sources with scalable and robust room-temperature quantum memories has been a long-standing challenge in photonic quantum information technologies due to inherent noise processes and time-scale mismatches between the operating conditions of solid-state and atomic systems. Here, we demonstrate on-demand storage and retrieval of single photons from a semiconductor QD device in a room-temperature atomic vapor memory. A deterministically fabricated InGaAs QD light source emits single photons at the wavelength of the cesium D1 line at 895 nm which exhibit an inhomogeneously broadened linewidth of 5.1(7) GHz and are subsequently stored in a low-noise ladder-type cesium vapor memory. We show control over the interaction between the single photons and the atomic vapor, allowing for variable retrieval times of up to 19.8(3) ns at an internal efficiency of 0.6(1)%. Our results significantly expand the application space of both room-temperature vapor memories and semiconductor QDs in future quantum network architectures.

15 min. break

HL 57.7 Fri 11:15 H13

Effects of atomistic fluctuations on the excitonic fine-structure in alloyed colloidal quantum Dots — •Anne Nadine Tewonoue Djota, Surender Kumar, and Gabriel Bester — Institute of physical chemistry and physics, University of Hamburg

The electron-hole exchange interaction in the presence of spin-orbit coupling leads for an atomistic calculation to a small energy splitting of the excitonic state known in this context as the fine structure splitting (FSS). Although this splitting is typically small, it has large consequences for the optical properties. For instance, the photoluminescence originates from these few states and is governed by the splitting (giving rise to temperature dependence) and polarization of these low energy excitonic states. So far most of the theoretical modeling has assumed that high symmetry structures lead to a simple dark-bright splitting with a large degeneracy of the excitonic states. In this work, we show based on atomistic calculations, that even globally perfectly symmetric structures (i.e., as far as an atomistic construction permits a "spherical" quantum dot) show a qualitatively different FSS as soon as alloying is introduced. The alloying effect is significantly stronger than any global shape anisotropy where the symmetry is broken for instance by geometrical elongation of the quantum dot. On the other hand, alloying a quantum dot through processes such as cation exchange is inherently random. As a result, different random alloy configurations with the same size and composition can exhibit significantly different FSS.

HL 57.8 Fri 11:30 H13

How Surface Defects Shape the Excitons and Photoluminescence of Ultrasmall CdSe Quantum Dots — •Torben Steenbock[1], Emilia Drescher[1], Tobias Dittmann[1], and Gabriel Bester[2,3] — [1]Department of Chemistry, University of Hamburg, HARBOR, Hamburg 22761, Germany. — [2]Department of Chemistry and Physics, University of Hamburg, HARBOR, Hamburg 22761, Germany. — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg 22761, Germany.

Ultrasmall CdSe quantum dots (QDs) with diameters up to 2 nm show broad photoluminescence (PL) spectra presumably due to emission from band-edge excitons and defect states. However, the origin of the defect emission and the effect of defects on the band-edge excitons is not fully understood. Based on spin-orbit density functional theory and screened configuration interaction singles, we show that Cd-dimer and Se defects form in-gap defect states. In comparison with experiment, we discuss the role of deep and shallow defect states for the PL and cover the dependence of their contributions to the PL with respect to the QD size. Further, we observe that these defects lead to a localization of the molecular orbitals (MOs) involved in the band-edge excitons creating large electric dipoles in the MOs. In the excitonic states, these dipoles cause multiexponential PL decay from the band-edge states with a highly anisotropic polarization of the emission. The polarization is found to be very sensitive with respect to the exact composition of the surface.

HL 57.9 Fri 11:45 H13

Room-temperature single photon emitters in hexagonal boron nitrite coupled to an open optical cavitiy — •Anthony Ernzerhof, Lukas Lackner, Martin Esmann, Ivan Solovev, and Christian Schneider — Carl von Ossietzky Universität Oldenburg, Germany

Single photon emitters (SPEs) are a key component in photonic quantum technologies. Potential applications include secure communications and quantum metrology. Here, we present SPEs at room temperature (RT) based on hexagonal boron nitride (hBN) nano crystallites, which exhibit remarkable optical properties[1]. Our work focuses on the integration of these SPEs in an optical cavity with open access and full tunability. The cavity device allows to enhance the emitter performance via the Purcell effect, which significantly improves the emitter emission rate and source collection efficiency[2]. We discuss our technological approach towards engineering the open cavity yielding a flexible, transportable, compact and userfriendly opto-mechanically tunable emitter-cavity device, which, in principle, is of universal use beyond hBN based single photon sources. We further discuss challenges associated to the implementation of hBN nano-crystallites in such a cavity.

[1] Tran, T.et al. Quantum emission from hexagonal boron nitride monolayers. Nature Nanotech 11, 37-41 (2016). [2] Tobias Vogl et al. Compact Cavity-Enhanced Single-Photon Generation with Hexagonal Boron Nitride, ACS Photonics 6 (8), 1955-1962 (2019).

HL 57.10 Fri 12:00 H13

Silicon nitride-based photonic integrated circuit interfaced via photonic wire bonds with InGaAs-QDs emitting at telecom wavelength — •Ulrich Pfister[1], Daniel Wendland[2,3], Florian Hornung[1], Lena Engel[1], Hendrik Hüging[2], Elias Herzog[1], Ponraj Vijayan[1], Raphael Joos[1], Erik Jung[3], Michael Jetter[1], Simone L. Portalupi[1], Wolfram H. P.

Pernice[2,3], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [3]Kirchhoff-Institute for Physics, University of Heidelberg, 69120 Heidelberg, Germany

Photonic integrated circuits (PICs) play a crucial role for realizing several quantum technologies in a small footprint. In this regard, hybrid approaches are beneficial for combining the highly developed silicon platform with the on-demand single-photon emission of III-V semiconductor quantum dots (QDs). We employed 3D laser writing technology to realize photonic wire bonds (PWBs) for funnelling single-photons from the III-V-based chip, containing the QDs emitting at 1550nm, into a Si_3N_4-based PIC [1]. An on-chip beamsplitter was used to measure a $g^{(2)}(0) = 0.11 \pm 0.02$, demonstrating the functionality of the hybrid approach on a single-photon level. Additionally, the average efficiency of the PWBs was precisely quantified.
[1] Ulrich Pfister, *et al.*, arXiv:2411.05647

HL 57.11 Fri 12:15 H13

Quantum Communication Protocols Using Polarization-Entangled Photon Emitters — Michele Rota[1], Francesco Basso Basset[1], •Francesco Salusti[2], Alessandro Laneve[1], Mattia Beccaceci[1], Giuseppe Ronco[1], Nicolas Claro Rodriguez[2], Thobias Krieger[3], Quirin Buchinger[4], Saimon Filipe Covre Da Silva[3], Sandra Stroj[5], Sven Höfling[4], Tobias Huber-Loyola[4], Armando Rastelli[3], Klaus Jöns[2], and Rinaldo Trotta[1] — [1]Department of Physics, Sapienza University of Rome, 00185 Rome, Italy — [2]PhoQS, CeOPP and Department of Physics, Paderborn University, 33098 Paderborn, Germany — [3]Institute of Semiconductor and Solid State Physics, JKU University, 4040 Linz, Austria — [4]Julius-Maximilians-Universität Würzburg, Physikalisches Institut, 97074 Würzburg, Germany — [5]Forschungszentrum Mikrotechnik, FH Vorarlberg, 6850 Dornbirn, Austria

We demonstrate entanglement swapping using [1] a quantum dot in a novel cavity with piezoelectric actuators [2]. We use these entan- gled photons after the swapping operation for quantum key distribu- tion with a modified Ekert91 protocol [3], highlighting temporal post- selection*s impact on photon indistinguishability and protocol metrics. References: [1] J.-W. Pan, et al., Phys. Rev. Lett. 80, 3891 (1998) [2] M. B. Rota, et al., eLight 4, 13 (2024), ISSN 2662-8643 [3] F. B. Basset, et al., Science Advances 7, eabe6379 (2021)

HL 57.12 Fri 12:30 H13

Efficient fiber coupling of telecom single photons from circular Bragg gratings — •Nam Tran[1], Pavel Ruchka[2], Sara Jakovljevic[2], Benjamin Breiholz[1], Peter Gierss[1], Ponraj Vijayan[1], Carlos Eduardo Jimenez[3], Alois Herkommer[3], Michael Jetter[1], Simone Luca Portalupi[1], Harald Giessen[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart — [2]4. Physikalisches Institut, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart — [3]Institut für Technische Optik, Research Center of Photonic Engineering, SCoPE, University of Stuttgart

This work aims at quantitatively investigating the spatial stability and coupling efficiency of telecom C-band photons, generated by an epitaxial quantum dot embedded in a circular Bragg grating, into single mode optical fibers. These results are then compared to a bare single mode fiber without the 3D printed lens and a collection via a microscope objective. In terms of the total fiber coupling efficiency, the lensed and bare fiber outperform the microscope objective by up to a factor of 2.9 corresponding to a measured count rate at the detectors of 0.44MHz and 1.11MHz, respectively. The lateral (vertical) displacement showed that within a few (a few tenths) of microns the coupling degrades less than a factor of two.

HL 57.13 Fri 12:45 H13

Development of Stark-tuned InGaAs quantum dots emitting in the telecom O-band on silicon substrate — •Sarthak Tripathi, Kartik Gaur, Imad Limame, Priyabrata Mudi, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

Quantum dots (QDs) are promising for single-photon emission, essen tial for quantum technologies like secure communication and quantum key distribution (QKD). In particular, InGaAs QDs that emit photons in the telecom O-band are especially valuable due to their compatibility with current metropolitan fiber-based QKD systems. Additionally, it is interesting to develop Si-compatible device concepts. Achieving High quality QDs on silicon are challenging due to lattice mismatch with III-V materials, leading to defects and performance degradation. To overcome this, we use a GaP buffer layer to reduce strain, improve lat tice matching, enabling high-quality QD growth with low defect den sities.By integrating epitaxial n- and p-doped GaAs layers with ohmic contacts, we apply an electric field to modify the QD energy levels via Stark effect, allowing controlled tuning of the emission wavelength. This tunability is crucial for aligning the QD emission with telecom standards or compensating for fabrication-induced variations. Optical and quantum optical characterizations confirm the effectiveness of this approach, demonstrating excellent quantum optical properties. These results highlight the potential of electrically tunable InGaAs QDs on Si as a scalable platform for quantum communication, compatible with Si-based technologies and fiber-based telecom networks.

HL 58: Nitrides: Preparation and Characterization II

Time: Friday 9:30–10:30 Location: H14

HL 58.1 Fri 9:30 H14

Random Alloy and Ordered Phases of Cubic Indium Gallium Nitride From a First-Principle Perspective — •Jan M. Waack[1,2], Markus Kremer[1,2], Nils Andre Schäfer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Although the miscibility gap in cubic zincblende indium gallium nitride ($In_xGa_{1-x}N$) has been overcome, the specific role of ordered phases in this process remains unclear. First-principle density functional theory calculations provide a reference point for addressing this question. Ordered phases, such as CuPt-type and chalcopyrite-type structures, exhibit unique structural and electronic properties that differentiate them significantly from the random alloy. An understanding of these distinctive features of ordered phases provides a basis for their experimental identification.

We present a comprehensive data set on key structural parameters, including lattice constants and bond lengths, as well as elastic properties such as elastic constants and phonon modes. Furthermore, we explore electronic properties including the band gap and Bloch spectral function using *ab-initio* approaches such as LDA-1/2 and the mBJ functional. The presented insights into the physical properties of ordered phases and the random alloy offer a robust foundation for their experimental detection and further exploration.

HL 58.2 Fri 9:45 H14

Characterization of structural and optical properties of a red InGaN/GaN MQW LED — •Niklas Dreyer[1], F. Bertram[1], G. Schmidt[1], H. Eisele[1], S. Petzold[1], O. August[1], A. Dempewolf[1], K. Wein[1], J. Christen[1], B. Sheng[2], and X. Wang[2] — [1]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [2]Peking University, Beijing 100871, China

An InGaN/GaN LED with an intended red emission (> 600 nm) was grown by MOVPE on a sapphire substrate. On an undoped GaN buffer followed by a doped n-GaN layer, the active region consists of a stack of three identical sequences, each with three quantum wells (QWs). The first two QWs nominally contain 15 % In (blue) and the third 40 % In (red). Each sequence is confined by an $Al_{0.32}Ga_{0.68}N$ layer. Finally, a p-doped $Al_{0.17}Ga_{0.83}N$ EBL is positioned, which is further capped by a dielectric DBR and processed, including metal contacts.

The LED is comprehensively characterized by cross-sectional cathodoluminescence performed in scanning transmission electron mi-

croscopy (STEM-CL) and by electroluminescence (EL). The luminescence along the growth direction is directly visualized in CL linescans: in particular, each QW can be spectrally and spatially resolved and shows a distinct emission. A wavelength shift for all QWs is observed. Furthermore, the n-GaN exhibits near-band-edge (NBE) luminescence at 356.7 nm at $T = 16$ K corresponding with a high free carrier concentration due to Burstein-Moss Shift.

The EL spectrum shows intense, broad emission around 650 nm, with a weak shift to shorter wavelengths for higher injection current.

HL 58.3 Fri 10:00 H14

Advanced nano-characterization of doped and undoped InGaN/GaN MQW-LED structures — •Luca Greczmiel, F. Bertram, G. Schmidt, P. Veit, H. Eisele, A. Dempewolf, S. Petzold, J. Christen, C. Berger, A. Dadgar, and A. Strittmatter — Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

In this study, we comprehensively investigate structural and optical properties of InGaN/GaN MQW-LED-structures by cathodoluminescence (CL) directly performed in a scanning transmission electron microscope (STEM). The LEDs are grown by MOVPE on top of an optimized GaN/sapphire template. The first pn-junction is formed by an 1.6 μm thick GaN:Si layer and a 345 nm thick GaN:Mg layer, which are nominally doped with a concentration of $7 * 10^{18}$ cm^{-3} and $2 * 10^{19}$ cm^{-3}, respectively. In between the n- and p-layer a MQW is located, which is composed of a stack of five InGaN QWs being separated by GaN:Si barriers, with a thickness of 3 nm and 7 nm, respectively. The InGaN wells have a nominal In content of 12 %. In STEM-linescans of the active region along the sample cross-section, the first QW shows emission at shorter wavelengths with respect to the subsequent following QWs. For comparison, a second MQW structure was investigated, which was identically grown, but sandwiched between uGaN. In contrast to the first sample, the CL of the 1st QW shifts to longer wavelengths, with respect to the subsequently following QWs. Hence, this spectral shift of the 1st QW is supposed to depend on the electric field in the space charge region.

HL 58.4 Fri 10:15 H14

Physical properties and thermal stability of zirconium platinum nitride thin films — Rebecca Gallivan[1], Ana Michelini[1], Nensi Toncich[1], Nerea Abando Beldarrain[1], Julia Manser[1], Arnold Müller[2], Christof Vockenhuber[2], and •Henning Galinski[1] — [1]Laboratory for Nanometallurgy, Department of Materials, ETH Zurich,8093 Zurich, Zurich, Switzerland — [2]Laboratory of Ion Beam Physics, Department of Physics, ETH Zurich, 8093 Zurich, Zurich, Switzerland

By providing new functionality, ternary transition metal nitrides (TMNs) have the potential to greatly broaden the material design space. Nevertheless, the majority of systems have only been studied computationally, and translation to experimental synthesis is restricted by a lack of knowledge about their stabilizing mechanisms. In this talk, we discuss the fabrication of ternary Zr-Pt-N thin films and examine their physical properties [1]. We show that Pt replaces nitrogen on the nonmetallic sublattice, destabilizing the rock salt structure and forming a complicated cubic phase. Additionally, we observe the exsolution of Pt nano precipitates from the Zr-Pt-N films upon annealing as well as degradation in the nitridic film's thermal stability. Even at low concentrations, Pt facilitates a solid reaction with the Si substrate that is otherwise inaccessible in ZrN films.

References: [1] Appl. Phys. Lett. 125, 221901 (2024)

HL 59: 2D Semiconductors and van der Waals Heterostructures VI

The sesssion covers the physics of interlayer excitons and allied phenomena in van der Waals heterostructures.

Time: Friday 9:30–11:45 Location: H15

HL 59.1 Fri 9:30 H15

Interlayer excitons in electric and magnetic fields — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Over the past years, more and more two-dimensional (2D) materials have been stacked to heterostructures. Due to the coupling interlayer excitations can form.

Here we report on a trilayer heterostructure of MoS_2 and WS_2. In contrast to bilayers, the coupling may lead to quadrupolar excitons. These can be clearly identified by the quadratic response of the corresponding excitons in our GW/BSE calculations in electric fields. In the second example, we report our studies of bulk CrSBr [1]. In a magnetic field the lowest bright excitations of the antiferromagnetically coupled CrSBr shift quadratically. Our calculations reveal the symmetry forbidden dark excitons and the increasing interlayer character. We develop a minimal model to explains this spin-dependent coupling. Despite its simplicity, the proposed model is generally applicable to any coupled 2D magnet.

[1] https://arxiv.org/abs/2403.20174

HL 59.2 Fri 9:45 H15

Signature of Rydberg-like states of interlayer excitons in MoSe2/WSe2 heterostructures — •Chirag Chandrakant Palekar[1], Paulo E. Faria Junior[2], Tobias Manthai[1], Maximilian Nagel[1], Bhabani Sankar Sahoo[1], Shachi Machchhar[1], Avijit Barua[1], Jaroslav Fabian[2], Barbara Rosa[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The heterostructures of transition metal dichalcogenides (TMDCs), formed by the stacking of different TMDC monolayers (MLs), facilitates the formation of spatially indirect interlayer excitons (IX). Due to the higher binding energy, the excited excitonic states have typically been observed in TMDC monolayers for over a decade. Nevertheless, the Rydberg-like higher-order states of the IX in WSe2/MoSe2 HSs have thus far remained undetected due to their weak oscillator strength. In this work, we employ photoluminescence excitation (PLE) spectroscopy to identify the signatures of Rydberg-like higher order states of IX in WSe2/MoSe2 HSs. By examining HSs with varying twist angles, we are able to gain comprehensive insight into the twist angle dependence of such excited states of IX. We compare experimental and theoretical results on the twist angle-dependent behavior of observed states, providing a systematic investigation that advances current understanding of the optical and electronic properties of TMDC HS systems.

HL 59.3 Fri 10:00 H15

Twisted MoSe2 Homobilayer Behaving as a Heterobilayer — •Arka Karmakar — Institute of Experimental Physics, Faculty of Physics, University of Warsaw, 02-093 Warsaw, Poland

Heterostructures (HSs) formed by the transition-metal dichalcogenides (TMDCs) materials have shown great promise in next-generation (opto)electronic applications. Traditionally, at atomically closed proximity the charge transfer (CT) process dominates due to its fast timescale ($<$ 50 fs). In this talk, I introduce our latest work [1] on the ET process in a twisted molybdenum diselenide (MoSe2) homobilayer without any charge-blocking interlayer, i.e., in atomically closed proximity. We fabricated an unconventional homobilayer (i.e., HS) with a large twist angle (~57°) by combining the chemical vapor deposition (CVD) and mechanical exfoliation (Exf.) techniques to fully exploit the lattice parameters mismatch and indirect/direct (CVD/Exf.) bandgap nature. These result in weakening the CT process and allowing the ET process to take over the carrier recombination channels. We employ a series of optical and electron spectroscopy techniques, complementing by the density functional theory (DFT) calculations, to describe a massive room temperature photoluminescence enhancement from the HS area due to an efficient ET process. Our results show that the electronically decoupled MoSe2 homobilayer is coupled by the ET process, mimicking a 'true' heterobilayer nature.

Reference: [1] A. Karmakar et al., "Twisted MoSe2 Homobilayer Behaving as a Heterobilayer", Nano Lett. 2024, 24, 31, 9459-9467.

HL 59.4 Fri 10:15 H15

Tailoring Interlayer Exciton Dyanamics of TMDC Heterostructures: From Bilayers to Trilayers embeded in Broadband DBR Cavities — •Bhabani Sankar Sahoo, Shachi Machchhar, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The photoluminescence yield of interlayer excitons (IX) at room temperature remains limited due to electrons and holes residing in different layers. In this work we propose and implement a novel way to enhance the IX emission in transition metal dichalcogenide (TMDC) heterostructures. We first introduce an additional WSe2 on top of a heterobilayers (HBL) of WSe2/MoSe2 to form a heterotrilayer (HTL) with different twist angles which significantly boost the PL emission upto one order magnitude, attributed to improved overlap of the electronic wavefunctions and additional radiative pathways. Further embedding this HTL within a chirped multiresonant distributed Bragg reflector (DBR) microcavity provides strong exciton confinement, enhancing the radiative recombination rate and modifying the exciton lifetime. Compared to the HBL, the HTL displays a reduced exciton lifetime, indicative of stronger light-matter coupling within the cavity, and a pronounced increase in PL intensity due to enhanced photon density of states. Our study highlights the potential of tailored stacking and cavity integration to manipulate light-matter interactions in advanced TMDC heterostructure devices for next-generation optoelectronic applications.

HL 59.5 Fri 10:30 H15

Effect of the Direct-to-Indirect Bandgap Crossover on the Reverse Energy Transfer — •Gayatri Gayatri[1], Debashish Das[2], Natalia Zawadzka[1], Takashi Taniguchi[3], Kenji Watanabe[3], Adam Babiński[1], Saroj K. Nayak[2], Maciej R. Molas[1], and Arka Karmakr[1] — [1]University of Warsaw, Warsaw, Poland — [2]Indian Institute of Technology Bhubaneswar, Odisha, India — [3]National Institute for Materials Science, Ibaraki, Japan

Heterostructures (HSs) made by the vertical stacking of van der Waals monolayers (1Ls) have shown great potential in (opto)electronic devices. In the type-II transition metal dichalcogenide HSs, long-range energy transfer (ET) happens via the dipole-dipole coupling (Förster type). To investigate this, we studied HS made by the 1L tungsten disulfide (WS2) and 1L-5Ls molybdenum disulfide (MoS2), with hexagonal boron nitride (hBN) as a charge-blocking interlayer, using differential reflection contrast, photoluminescence (PL), and photoluminescence excitation. At room temperature, PL enhancement has been observed in the neutral exciton of WS2 in the WS2-hBN-1L MoS2 and WS2-hBN-2L MoS2 regions as compared to the isolated WS2 emission. This enhancement confirms an efficient ET from MoS2 B excitonic level to WS2 A excitonic level. As the number of MoS2 layers increases, bandgap changes from direct-to-indirect, promoting more immediate carrier scattering from the K-valley. Consequently, carrier population decreases and ET becomes less effective.

HL 59.6 Fri 10:45 H15

Interlayer Exciton Traps in TMD heterobilayers — •Thomas Klokkers[1,2], Mirco Troue[1,2], Johannes Figueiredo[1,2], Andreas Knorr[3], Ursula Wurstbauer[4], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany — [3]Institute for Theoretical Physics, Nonlinear Optics and Quantum Electronics, Technical University of Berlin, 10623 Berlin, Germany — [4]Institute of Physics, Münster University, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Long-lived interlayer excitons in MoSe2/WSe2 heterostructures constitute a promising platform to explore many-body physics in a two-dimensional solid-state system. Introducing a trapping potential facilitates exploring the many-body regime by providing a platform to control the density of the interlayer exciton ensemble. Realizations of such exciton traps range from electrostatic strip gates to strain-induced potentials. In this work, we realize enhanced emission from interlayer excitons based on an optical trap. The laterally changed potential landscape allows the investigation of ensembles at high densities without the direct influence of temperature, excess charge carriers and laser-induced coherence.

15 min. break

HL 59.7 Fri 11:15 H15

Hybridized excitons in 2D van der Waals materials — •Andreas Stier — Walter Schottky Institut und TUM School of Natural Sciences, TU München, Garching, Deutschland

I will review our recent progress on magneto optical spectroscopy of atomically thin materials in magnetic fields up to 91 T with an emphasis on the spin-valley physics of neutral and charged excitons.

In monolayer (ML) semiconductors, magneto-absorption spectroscopy revealed the diamagnetic shifts of the exciton Rydberg states, which allowed the first direct experimental measure of the reduced mass and binding energy. Surprisingly, investigating the photoluminescence, we observe the emergence of a new excitonic peak, which we discuss in the framework of the theoretically predicted linear dispersing exciton branch originating from intervalley exchange interactions.

For heterostructures (HS) of a 2D semiconductor with graphene, we find a new multi-step proximity effect due to band folding in the HS, where we show that the spin-valley physics can be used to quantify interlayer hybridization. In HS from ML MoSe2 and the layered antiferromagnetic (AFM) semiconductor CrSBr, we show the formation of new exciton states depending on the twist angle. These excitons exhibit clear signatures of proximity coupling to the magnetic state of the AFM layer, such as hysteretic response to in- and out of plane B fields. We discuss these results in the framework of Ising-type spin-orbit proximity coupling.

HL 59.8 Fri 11:30 H15

Laterally extended states of interlayer excitons in reconstructed $MoSe_2/WSe_2$ heterostructures — •Johannes Figueiredo[1,2], Marten Richter[3], Mirco Troue[1,2], Jonas Kiemle[1,2], Hendrik Lambers[4], Torsten Stiehm[4], Ursula Wurstbauer[4], Andreas Knorr[3], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]Munich Center for Quantum Science and Technology (MCQST) — [3]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin — [4]Institute of Physics, Münster University

Heterostructures made from 2D transition-metal dichalcogenides are ideal platforms for exploring excitonic phenomena, including correlated moiré excitons and degenerate interlayer exciton ensembles. While atomic reconstruction is often assumed to localize excitons, we demonstrate that excitonic states in reconstructed $MoSe_2/WSe_2$ heterostructures can extend beyond the moiré periodicity [1]. Using real-space calculations, we provide lateral potential maps and corresponding excitonic wavefunctions for interlayer excitons in strain-relaxed heterostructures [2]. Cryogenic photoluminescence experiments corroborate the computed level structure and exciton relaxation dynamics. These findings align with recent coherence measurements on degenerate interlayer excitons and suggest potential many-body phenomena in dense, cold exciton ensembles [3].

[1] J. Figueiredo et al., arXiv:2411.19616 (2024) [2] M. Richter, PRB 109, 125308 (2024) [3] M. Troue and J. Figueiredo et al., PRL 131, 036902 (2023)

HL 60: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)

The joint focus session of the divisions HL and MA presents the latest developments of the rapidly growing community working with the van der Waals magnetic semiconductor CrSBr with distinct excitonic and magnetic properties, and it is organized by Shengqiang Zhou (HZ Dresden-Rossendorf), Farsane Tabata-Vakili (TU Braunschweig), and Florian Dirnberger (TU Munich).

Time: Friday 9:30–13:00 Location: H17

Invited Talk HL 60.1 Fri 9:30 H17

Constructing Artificial Matter in the Electron Microscope - Atomic Fabrication at Scale in CrSBr — •Julian Klein — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

The ability to control the arrangement of individual atoms has transcended naturally occurring configurations of matter, enabling experimental breakthroughs in quantum physics. I will show how we can now use scanning transmission electron microscopy to construct artificial atomic arrangements at scale and demonstrate it with the layered magnetic quasi-1D semiconductor CrSBr. By developing strategies to position the electron beam with picometer precision and perform rapid, targeted beam actions, we achieve deterministic control over the movement of Cr atoms in space and time. With this capability, we selectively steer Cr atoms into interstitial positions, forming localized quantum states while simultaneously monitoring atomic movements in real time with microsecond resolution. Fully automating the electron microscope enables us to construct ordered arrays of Cr interstitial superlattices atom by atom as well as nonperiodic structures, spanning hundreds of locations over tens of nanometers, all within minutes. Our results show that atomic fabrication at scale in the electron microscope is now a reality, unlocking unprecedented opportunities to construct quantum defects and phases, atom by atom, in the solid state, that extend over macroscopic length scales.

Invited Talk HL 60.2 Fri 10:00 H17

Tuning the structure and magnetism in CrSBr via external pressure — •Ece Uykur — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

As one of the two-dimensional (2D) van der Waals (vdW) magnets, CrSBr regained significant attention recently because it is air-stable even in the monolayer form making this compound very attractive. It shows strong coupling between its magnetic, electronic, structural, and optical properties [1]. Several ab initio calculations put forward the importance of the balance between Cr-Cr direct exchange and Cr-anion-Cr superexchange interactions and showed that the A-type antiferromagnetism in this compound is delicately balanced with these short- and long-range magnetic interactions [2]. Therefore, studies exploring the tunability of the inter- and inralayer coupling are important and one plausible experimental strategy is the external pressure.

In this talk, I will summarize our recent efforts on high-pressure single crystal XRD and magnetization studies on CrSBr. We performed single crystal XRD studies up to ∼20 GPa, which reveals a non-monotonous behavior of Cr-ion in the structure along with a structural phase transition above 17 GPa. The movement of this Cr-ion has also direct link with the magnetization of the compound that is studied with the high-pressure magnetic susceptibility measurements up to ∼8 GPa.

[1] K. Lin et al., ACS Nano 18, 2898 (2024) [2] J. Cenker et al., Nat. Nanotechnol. 17, 256 (2022).

Invited Talk HL 60.3 Fri 10:30 H17

A theoretical perspective on exciton-magnon coupling and its implications — •Akashdeep Kamra — Department of Physics, Rheinland-Pfälzische Technische Universität (RPTU) Kaiserslautern-Landau, Kaiserslautern, Germany

The dependence of exciton energies on the magnetic order in CrSBr has opened avenues for controlling optical properties using magnetic fields. Conversely, it has enabled an optical time-resolved sensing of the magnetic degrees of freedom. This has further been exploited to investigate the interplay between excitons and magnons, the excitations of the magnetic order. We will discuss how excitonic energies offer a convenient access to coherent as well as thermal magnon dynamics. Focusing on transport, we will discuss the recent observation of the magnon-exciton drag effect that makes it feasible to leverage thermal magnon currents for transporting excitons at unexpectedly fast velocities. Finally, we will conclude with a brief discussion of emergent non-linearities in exciton energies mediated by the magnonic modes in the canted magnetic state of CrSBr.

References:

1. F. Dirnberger et al., Magneto-optics in a van der Waals magnet tuned by self-hybridized polaritons, Nature 620, 533 (2023).

2. F. Dirnberger, S. Terres, Z. A. Iakovlev, K. Mosina, Z. Sofer, A. Kamra, M. M. Glazov, and A. Chernikov, Exciton transport driven by spin excitations in an antiferromagnet (unpublished).

3. B. Datta et al., Magnon-mediated exciton-exciton interaction in a van der Waals antiferromagnet, arXiv:2409.18501.

15 min. break

Invited Talk HL 60.4 Fri 11:15 H17

Exciton and valley properties of monolayer transition metal dichalcogenides on the van der Waals magnetic semiconductor CrSBr — •Yara Galvao Gobato — Universidade Federal de Sao Carlos, Sao Carlos, Brazil

Chromium sulfide bromide is a promising van der Waals (vdW) magnetic material, undergoing a magnetic phase transition to an A type antiferromagnetic state below the Neél temperature of about 132K in its bulk form. VdW heterostructures composed of monolayer transition metal dichalcogenides (TMDs) and vdW magnetic materials such as CrSBr are an interesting platform to modify valley and excitonic properties of non-magnetic TMDs. In this talk, we will present our recent results on optical and magneto-optical properties of monolayer TMDs on CrSBr under different magnetic field orientations. Remarkably, we have observed a clear influence of the CrSBr magnetic order on the exciton and valley properties of monolayer TMDs, such as an anomalous linear polarization dependence, unsual temperature dependence of emission energies, magnetic field dependence of the emission intensity, and valley g-factor values with clear signatures of an asymmetric magnetic proximity exchange interaction. Our results are explained by asymmetric magnetic proximity effects, charge transfer and a possible contribution of exciton/trion magnon coupling. Our studies suggest that vdW heterostructures with antiferromagnetic nonmagnetic interfaces are interesting platforms to modify the valley and excitonic properties of TMDs for possible applications in opto-spintronics and quantum technology.

HL 60.5 Fri 11:45 H17

Ab initio studies on the electronic and optical properties of magnetic CrSBr — •Marie-Christin Heissenbüttel[1], Pierre-Maurice Piel[2], Julian Klein[3], Thorsten Deilmann[1], Ursula Wurstbauer[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Physical Institute, University of Münster, Germany — [3]Department of Materials Science and Engineering, MIT, Massachusetts, USA

CrSBr recently emerged as a van der Waals layered material exhibiting intriguing electronic and optical properties arising from the intricate interplay between crystal structure and layered magnetic order. A thorough understanding of these effects is essential to assess its potential for applications in spintronic and quantum devices. Due to the large crystal anisotropy, the monolayer, multilayer, and bulk crystal CrSBr show a quasi-one-dimensional behaviour of effective masses and exciton wavefunctions [1]. The interlayer antiferromagnetic (AFM) coupling suppresses layer to layer interactions in the magnetic ordered low temperature phase, resulting in strong quantum confinement of electrons and excitons within the individual layers [2]. Using ab-initio GW/Bethe-Salpeter equation calculations, we analyze electronic and excitonic properties on the same footing and elucidate how the AFM van der Waals stacking, symmetry properties and the large crystal

anisotropy govern the electronic and optical properties of this material.

[1] https://doi.org/10.1021/acsnano.2c07316
[2] https://doi.org/10.48550/arXiv.2403.20174

HL 60.6 Fri 12:00 H17

Internal structure and ultrafast dynamics of quasi- 1D excitons controlled by magnetic order — •N. Nilforoushan[1], M. Liebich[1], M. Florian[2], F. Mooshammer[1,3], A. D. Koulouklidis[1,3], L. Wittmann[1], K. Mosina[4], Z. Sofer[4], F. Dirnberger[5], M. Kira[2], and R. Huber[1,3] — [1]Dept. of Physics, University of Regensburg, Germany — [2]Dept. of Electrical Engineering and Computer Science, University of Michigan, USA — [3]RUN, University of Regensburg, Germany — [4]Dept. of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [5]Dept. of Physics, Technical University of Munich, Germany

In van der Waals (vdW) layered crystals, Coulomb correlations are often tuned by structural engineering, giving rise to emergent phenomena such as tightly bound excitons and exotic electronic and magnetic phases. Magnetic vdW materials offer a unique platform for in situ control of Coulomb correlations enabled by their intrinsic magnetic order. Here, we present quantitative experiment-theory proof that excitonic correlations can be tailored through spin order in the vdW magnet CrSBr. By probing internal transitions of excitons with phase-locked mid-infrared pulses, we reveal their binding energy and strong anisotropy of their quasi-1D orbitals resulting in significant fine-structure splitting. We switch excitons from monolayer-localized to interlayer-delocalized species by pushing the system from the antiferromagnetic to the paramagnetic phase. The exciton's ultrafast dynamics further support this scenario. In future applications, excitons may be interfaced with spintronics enabling on-demand phase transitions.

HL 60.7 Fri 12:15 H17

Raman controlled lithium intercalation into CrSBr van der Waals structure — •Ksenia Mosina, Aljoscha Söll, Martin Veselý, Jiří Šturala, and Zdenek Sofer — Department of Inorganic Chemistry, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic.

Lithium intercalation into the van der Waals crystalline structure of layered transition metal dichalcogenides by means of chemical and electrochemical intercalation is a well-known method for studying semiconductor-metallic phase transitions. The layered semiconductor chromium sulphur bromine (CrSBr) in recent years becomes an ultimate playground for the studies of low-dimensional magneto-optical properties. The interlayer distance of CrSBr allows the easy cleavage and intercalation of the guest molecules within the crystalline structure. Conveniently air-stable, this material exhibits a direct band gap of 1.5 eV, an antiferromagnetic state in bulk and ferromagnetism in the monolayer. Here, we present the lithium intercalation method into the CrSBr structure by lithium-solvated electron solution. To monitor the lithiation process in real-time, we investigated the Raman spectra evolution upon lithium ion intercalation into a few-layered CrSBr flake. Our findings suggest that the quasi-one dimensional nature of CrSBr leads to weak interlayer hybridization along the b-direction, which facilitates the diffusion of guest ions by lowering the migration energy barrier and enables anisotropic Li+ diffusion. The reliable intercalation methodology allows tracking the intercalation process directly in the desired area favorable for device fabrication.

Invited Talk HL 60.8 Fri 12:30 H17

Electric field control of intra- and interlayer excitons in CrSBr — •Nathan Wilson[1], Amine Ben Mhenni[1], Ferdinand Menzel[1], Alain Dijkstra[1], Zdenek Sofer[2], and Jonathan Finley[1] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]Institute of Chemistry and Technology, Prague, Czech Republic

In the 2D magnetic semiconductor CrSBr, the interplay between a direct bandgap for all layer thicknesses and layered antiferromagnetism with strong magneto-electronic coupling give rise to rich but poorly understood excitonic physics. So far, the presence of two closely spaced conduction bands and existence of both intra and interlayer excitons in multilayers has complicated interpretation of the optical spectrum of its excitons. Here, we study monolayers and bilayers of CrSBr in dual-gated structures, allowing for independent tuning of electric field and charge doping. Our study reveals the existence of the previously unobserved ground state exciton in monolayers, which is darkened both by charge doping and electric field. We find that both intralayer and hybrid intra/interlayer excitons are highly sensitive to the vertical electric field, implying a reasonably large exciton polarizability and control over wavefunction symmetry. With this information, we are able to form a more complete picture of the real space and band character of the excitons in CrSBr.

HL 61: THz and MIR physics in semiconductors

The session covers the THz and MIR physics in semiconductors.

Time: Friday 10:45–11:45 Location: H14

HL 61.1 Fri 10:45 H14

Multi-photon Stark spectroscopy of ultrafast THz waveforms — •Fabian Brütting, Moritz B. Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Microscopic electric waveforms can be encoded into luminescence modulations through the quantum-confined Stark effect, enabling ultrafast "videography" of local electric fields up to THz frequencies. This technique, known as Quantum-probe field microscopy (QFIM), relies on the coupling of momentary electric fields with electronic transitions in colloidal quantum dots, with detection achieved via pump-probe microscopy [1].

Here, we propose two-photon absorption (TPA) as a novel probing regime for accessing the THz-driven Stark effect. Unlike conventional Stark spectroscopy, which relies on linear one-photon absorption, TPA operates under different selection rules, resulting in distinct interaction dynamics. In particular, depending on the specific transitions being probed, we observe a sign flip of the nonlinear electro-absorption contribution relative to the linear signal. Consequently, the overall electro-absorption signal is either enhanced, reduced or even inverted compared to the linear signal.

Therefore, two-photon Stark spectroscopy offers potential for improving QFIM detection sensitivity and provides a novel strategy for the ultrafast manipulation of the optical properties in low-dimensional semiconductors.

[1] Heindl, Moritz B., et al. "Ultrafast imaging of terahertz electric waveforms using quantum dots." *Light Sci. Appl.* 11.1 (2022): 5.

HL 61.2 Fri 11:00 H14

Characterization of SiC epilayers with terahertz time-domain spectroscopy — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Christian Röder[3], Franziska Beyer[3], Kuei-Shen Hsu[4], Jan Beyer[4], Nadine Schüler[5], Nico Vieweg[6], Katja Dutzi[6], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department of Materials Characterization and Testing, Fraunhofer ITWM, Kaiserslautern — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau — [3]Department Energy Materials and Test Devices, Fraunhofer IISB, Erlangen — [4]Institute of Applied Physics, Technische Universität Bergakademie Freiberg — [5]Freiberg Instruments GmbH, Freiberg — [6]TOPTICA Photonics AG, Gräfelfing

Silicon carbide (SiC), being a wide-bandgap and robust, temperature-stable semiconductor, is an up-and-coming material that already has applications in power electronics and in high-temperature environments. While the characterization of the electrical and optical properties of bulk semicondcutors with terahertz time-domain spectroscopy (TDS) has already been demonstrated, many applications make use of thin layers with thicknesses of a few tens of microns. Using the Drude model, we performed simulations with varying thicknesses and charge carrier densities of SiC epilayers showcasing the opportunities and possible limitations of TDS to characterize SiC epilayers. Finally, TDS measurements demonstrating the validity of the simulations were used to determine the charge carrier density of SiC epilayers.

HL 61.3 Fri 11:15 H14

Diminishing topological Faraday effect in thin layer samples — Christian Berger, Florian Bayer, Laurens W. Molenkamp, and •Tobias Kiessling — Physikalisches Institut, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

A striking feature of three-dimensional topological insulators (TIs) is the theoretically expected topological magnetoelectric (TME) effect, which gives rise to additional terms in Maxwell's laws of electromagnetism with an universal quantized coefficient proportional to half-integer multiples of the fine-structure constant. In an ideal scenario one therefore expects also quantized contributions in the magnetooptical response of TIs.

We review this premise by taking into account the trivial dielectric background of the TI bulk and potential host substrates, and the often present contribution of itinerant bulk carriers. We show (i) that one obtains a nonuniversal magnetooptical response whenever there is impedance mismatch between different layers and (ii) that the detectable signals due to the TME rapidly approach vanishingly small values as the impedance mismatch is detuned from zero.

HL 61.4 Fri 11:30 H14

Unraveling the Microscopic Mechanism of Displacive Excitation of Coherent Phonons in a Bulk Rashba Semiconductor — •Peter Fischer[1], Julian Bär[1], Moritz Cimander[1], Volker Wiechert[1], Oleg Tereshchenko[2], and Davide Bossini[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]Nowosibirsk, Russia

Optically driven lattice excitations have recently been intensively investigated as a means to manipulate the macroscopic properties of quantum materials. In solids with an electronic band gap, it is well-established that coherent phonons can be excited by laser pulses with photon energies exceeding the band-gap energy. However, the dominant microscopic mechanism has still not been pinpointed: Neither experimentally nor theoretically has it been possible to disentangle the effect of a photo-induced change in the charge-carrier density from an increase of the carrier temperature. We perform time-resolved pump-probe spectroscopy on the Rashba semiconductor BiTeI. Tuning the pump-photon energy from the visible to the mid-infrared allows us to excite both interband and barely accessible intraband transitions. As a result, we determine that the lattice modes are mainly driven by the increased carrier temperature. In addition, the phonon coherence time in the intraband regime proves robust against an increase in laser fluence. These findings provide new insights for the development of schemes addressing the coherent structural manipulation of solids.

HL 62: 2D Semiconductors and van der Waals Heterostructures VII

The session covers the physics of quantum emitters and defects in 2D materials and their heterostructures. Note, the session starts directly after the session "2D Semiconductors and van der Waals Heterostructures VI".

Time: Friday 11:45–13:00 Location: H15

HL 62.1 Fri 11:45 H15

Deterministic Purcell enhancement of single photon emission from a WSe_2 monolayer quantum emitter — •Ivan Solovev[1], Victor Mitryakhin[1], Sven Stephan[1,2], Jens-Christian Drawer[1], Lukas Lackner[1], Seth Tongay[3], Kenji Watanabe[4], Takashi Taniguchi[5], Martin Esmann[1], and Christian Schneider[1] — [1]Institute for Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [2]University of Applied Sciences Emden/Leer, Emden, Germany — [3]Materials Science and Engineering, School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona, USA — [4]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Bright and easily fabricated quantum emitters in two-dimensional semiconductors have emerged as a promising platform for scalable quantum communication [1,2]. Here, we show, how their performance can be markedly elevated by integrating a monolayer into a versatile open plano-concave Fabry-Pérot microcavity. We managed to modulate radiative decay rate of a zero-phonon line by tuning a high Q-factor cavity. Reached five-fold shortening of the lifetime opens the route towards higher rates of quantum key distribution and generation of indistinguishable single photons in 2D semiconductors.

[1] J.C. Drawer et al., Nano Lett. 23 (18), 8683 (2023). [2] T. Gao et al. npj 2D Mater Appl 7, 4 (2023).

HL 62.2 Fri 12:00 H15

Deterministic generation of single-photon emitters in 2D materials by in-situ electron beam lithography — •Shachi Machchhar, Bhabani Sankar Sahoo, Yuhui Yang, Imad Limame, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The development of on-demand sources of single photons with high indistinguishability represents a crucial step in the creation of photonic quantum systems, such as those required for the construction of large-scale quantum networks for the secure transfer of data. One potential avenue for the realization of such sources in a scalable and cost-effective manner is the exploitation of defect centres in transition metal dichalcogenides (TMDCs). The fabrication of these defect centres in TMDC monolayers can be achieved through the introduction of strain, ion implantation, and the structuring or patterning of the substrate. In this study, we employ cathodoluminescence (CL) spectroscopy at cryogenic temperatures to probe hBN-encapsulated WSe* and utilise in-situ electron beam lithography (iEBL) to structure predetermined patterns on the emission active region. This nanopatterning of the monolayer facilitates the deterministic generation of single-photon emitters (SPEs) with distinct quantum optical properties. Furthermore, we demonstrate the single-photon nature of these SPEs through second-order correlation measurements on the MLs. Additionally, we study the temperature dependence of such SPEs generated in various patterned geometries.

HL 62.3 Fri 12:15 H15

Generation of luminescent defects in hBN by focused helium ion beam irradiation — •Amedeo Carbone[1,2], Martijn Wubs[1], Alexander W. Holleitner[2], Christoph Kastl[2], Alexander Huck[3], and Nicolas Stenger[1] — [1]Department of Electrical and Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]Walter Schottky Institute, Physik Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [3]Center for Macroscopic Quantum States (bigQ), Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Among the luminescent centres in hBN, which have recently gained attention because of their brightness and exceptional quantum properties at room temperature, the charged boron vacancy ($V_{\overline{B}}$) defect stands out for its magnetic properties, which have significant applications in quantum sensing schemes [1]. In the present work [2] we irradiate hBN flakes with a focused helium ion beam to generate $V_{\overline{B}}$ defects, conduct optical and magnetically resolved characterization, and apply a theoretical model [3] to infer the generated density of charged emitters. These results are further compared to the estimated vacancy density from Molecular Dynamics simulations. Our work provides a systematic study of the defect generation efficiency by comparing different irradiation doses.

[1] Gottscholl, A. et al., *Nat. Mater.* 19, 540-545 (2020), [2] Carbone, A. et al., *in preparation*, [3] Udvarhelyi, P. et al., *npj Comp. Mat.* 9, 150 (2023).

HL 62.4 Fri 12:30 H15

Impact of low-energy ion-irradiation induced defects on optical and vibrational properties of molybdenum disulfide — •Philipp Kraus, Eileen Schneider, Tobias Dierke, Stefan Wolff, Yuri Koval, and Janina Maultzsch — Chair of Experimental Physics, FAU Erlangen-Nürnberg, Erlangen

We present the controlled creation of vacancies in 2D materials, in par-

ticular graphene and molybdenum disulfide (MoS_2), by low-energy ion-irradiation. With Raman spectroscopy on exfoliated graphene flakes before and after irradiation, we determined the defect density to calibrate the ion dose of our setup. Then, we irradiated MoS_2 monolayers, grown via chemical vapor deposition (CVD), and determined the impact of the ion-induced defects on Raman and photoluminescence (PL) spectra. These results are additionally compared with density functional theory (DFT) calculations.

HL 62.5 Fri 12:45 H15

Composition- and strain-dependent quantum dot states in transition metal dichalcogenide nanobubbles — •Stefan Velja, Jannis Krumland, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Mechanical deformations in transition metal dichalcogenide monolayers can appear both spontaneously and artificially, giving rise to peculiar nanostructures, such as nanobubbles, or nanowrinkles. These systems have been observed to harbor localized states in the gap region, a known prerequisite for single-photon emission. While recent theoretical studies have attempted to explain these phenomena on selected systems [1,2], a detailed analysis concomitantly examining the role of the chemical constituents and the amount of applied strain is essential to gain full insight. In this work, we investigate the electronic properties of MX_2 nanobubbles (M=Mo, W and X=S, Se) characterized by varying levels of local strain. For materials composed of lighter elements, localized states appear in the gap region when the deforming force reaches the order of 0.01 a.u./atom. A thorough analysis of these states sets the stage for predicting and interpreting the optical fingerprints of these nanostructures.

[1] Krumland et al., *ACS Photonics* **11**, 586 (2024)
[2] Velja et al., *Nanoscale* **16**, 7134 (2024)

HL 63: Focus Session: Nanoscale Light-matter Interaction II

The focus session highlights recent breakthroughs in resolving the optoelectronic properties of individual nanostructures down to the atomic scale. Moreover, the session introduces the rich field of surface polaritons, confined electromagnetic modes through which light can be guided on subwavelength scales.

The session is the second part of the focus session on nanoscale light-matter interaction.

Time: Friday 12:00–13:15 Location: H14

HL 63.1 Fri 12:00 H14

Super-resolution imaging of nanoscale inhomogeneities in hBN-covered and encapsulated few-layer graphene — •Lina Jäckering, Konstantin G. Wirth, Lukas Conrads, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Encapsulating few-layer graphene (FLG) in hexagonal boron nitride (hBN) can cause nanoscale inhomogeneities in the FLG, including changes in stacking domains and topographic defects.[1] Due to the diffraction limit, characterizing these inhomogeneities is challenging. Recently, the visualization of stacking domains in encapsulated four-layer graphene (4LG) has been demonstrated with phonon polariton (PhP)-assisted near-field imaging.[2] However, the underlying coupling mechanism and ability to image subdiffractional-sized inhomogeneities remain unknown. Here, we retrieve direct replicas and magnified images of subdiffractional-sized inhomogeneities in hBN-covered trilayer graphene (TLG) and encapsulated 4LG, enabled by the hyperlensing effect.[3] This hyperlensing effect is mediated by hBN*s hyperbolic PhP that couple to the FLG*s plasmon polaritons. Using near-field microscopy, we identify the coupling by determining the polariton dispersion in hBN-covered TLG to be stacking-dependent. Our work demonstrates super-resolution and magnified imaging of inhomogeneities, paving the way for the realization of homogeneous encapsulated FLG transport samples to study correlated physics.

[1] Geisenhof et al. ACS Appl. Nano Mater. **2**, 6067 (2019). [2] Liu et al. Nat. nanotech. **19**, 188-195 (2024). [3] Li et al. Nat. Commun. **6**, 7507 (2015).

HL 63.2 Fri 12:15 H14

Optical and Electrical Properties of Copper Oxide * Polyvinyl Alcohol Nanocomposites for Solar Cell Applications — •Ahed AL-Faouri[1,2], Mahmoud Abu-Kharma[1], and Mahmoud Hatem[1] — [1]Department of Physics, Faculty of Science, Al-Balqa Applied University, Al-Salt, Jordan — [2]Basic Sciences Department, Faculty of Arts and Sciences, Al-Ahliyya Amman University, Amman, Jordan

Copper oxide nanoparticles (CuO-NPs) were successfully synthesized at ambient temperature using an easy and eco-friendly method, employing the aqueous extract of bougainvillea leaves as reducing and stabilizing agents. First, a thin film of pure polyvinyl alcohol (PVA) was prepared via solution casting. Subsequently, four CuO-PVA nanocomposites were fabricated through solution casting at concentrations of (13, 30, 40, and 51) wt%. The optical and electrical properties of the synthesized CuO NPs, pure PVA, and CuO-PVA thin films were investigated using a UV-Vis spectrophotometer and a Keithley electrometer.

The band gap (Eg) of prepared CuO-NPs was 2.74 eV. The separation of this band gap renders CuO-NPs a suitable material for solar energy conversion and could potentially be used as an active layer material in solar cells., Furthermore, the four prepared CuO-PVA showed that the optical band gap decreased from 4.42 eV (pure PVA) to 3.34 eV (50%CuO-PVA). Further, increased DC electric conductivity was observed

HL 63.3 Fri 12:30 H14

Accessing phase and group velocities of terahertz surface plasmon polaritons in graphene using near-field spacetime imaging — •Simon Anglhuber[1], Martin Zizlsperger[1], Eva A. A. Pogna[2], Yaroslav A. Gerasimenko[1], Anastasios D. Koulouklidis[1], Imke Gronwald[1], Svenja Nerreter[1], Leonardo Viti[3], Miriam S. Vitiello[3], Rupert Huber[1], and Markus A. Huber[1] — [1]Regensburg Center for Ultrafast Nanoscopy (RUN) and Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerche (CNR-IFN), Milano, I-20133, Italy — [3]NEST, CNR - Istituto Nanoscienze and Scuola Normale Superiore, Piazza San Silvestro 12, 56127, Pisa, Italy

The combination of light and matter properties in surface polaritons offers unprecedented opportunities for controlling energy flow and information processing at the nanoscale. Here, we present a novel THz near-field imaging approach to visualize polariton propagation directly in the time domain. Our method allows for the extraction of phase and group velocities, as well as damping. Thus, it reveals substantial insights into the polariton dispersion curve, even for strongly damped modes. Additionally, we show that our analysis can be expanded to two dimensions, directly visualizing polariton propagation in arbitrary directions, which is especially valuable for anisotropic materials. Finally, the method offers an intuitive approach to visualize non-equilibrium polariton propagation, e.g. upon photoexcitation. Thereby, we achieve subcycle control over polariton dynamics.

HL 63.4 Fri 12:45 H14

Inelastic electron-light interaction probed by holographic scanning transmission electron microscopy — •Nora Bach[1,2], Tim Dauwe[1,2], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Quantitative phase-contrast imaging of electrostatic potentials is an important application in transmission electron microscopy. Recently developed techniques have overcome the challenge to measure phase profiles inherited from optical fields, but offer only limited variability in tailoring the electron-light interactions and require a highly coherent electron source [1,2]. In this contribution, we introduce scanning transmission electron microscopy with spatially separated coherent electron probes [3] for the full imaging of complex optical near fields at a nanostructure with high spatial resolution. In the far field, these electron probes interfere to form a hologram from which we reconstruct phase

shifts induced both by elastic scattering processes and by stimulated inelastic interactions. One particular advantage of STEM holography is the relaxed coherence requirements, which could be central to improving time-resolved imaging of electric and magnetic fields on the nanoscale.

[1] Gaida et al., Nat Commun. 14, (2023)
[2] Gaida et al., Nat. Photon. 18 (2024)
[3] Fehmi et al., J. Phys. D: Appl. Phys. 51 (2018)

HL 63.5 Fri 13:00 H14

Unraveling ultrafast exciton dynamics in a monolayer of the magnetic semiconductor CrSBr — •Jakob Schlosser[1], Christian Meineke[1], Martin Zizlsperger[1], Marlene Liebich[1], Nilofar Nilforoushan[1], Kseniia Mosina[2], Sophia Terres[3], Alexey Chernikov[3], Zdenek Sofer[2], Markus A. Huber[1], Matthias Florian[4], Mack Kira[4], Florian Dirnberger[3], and Rupert Huber[1] — [1]University of Regensburg, Regensburg — [2]University of Chemistry and Technology Prague, Prague — [3]Dresden University of Technology, Dresden — [4]University of Michigan, Ann Arbor

Among van der Waals semiconductors, CrSBr stands out as both its bulk and monolayer forms host tightly bound, quasi-1D excitons in a magnetic environment. Despite the strong attention these quasiparticles have attracted, their lifetimes remained unknown. Terahertz spectroscopy can directly probe the dynamics of all electron-hole pairs, independently of interband selection rules. Yet the corresponding far-field foci substantially exceed the lateral sample dimensions. Here, we combine terahertz polarization spectroscopy with near-field microscopy to study the dynamics of bound and unbound electron-hole pairs in bulk CrSBr and extract the nonequilibrium dielectric function of the monolayer in a model-free manner. Interestingly, the femtosecond decay of paramagnetic excitons in monolayer CrSBr is found to be 30 times shorter than the determined lifetime in bulk material. Our results mark the first direct access to the ultrafast dielectric response of quasi-1D excitons in CrSBr, to advance the development of quantum devices based on ultrathin van der Waals magnets.