# Semiconductor Physics Division
# Fachverband Halbleiterphysik (HL)

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## Overview of Invited Talks and Sessions

(Lecture halls EW 201, EW 202, EW 203, EW 015, EW 561, and ER 325; Posters E and F)

### Invited Talks

| | | | | |
|---|---|---|---|---|
| HL 1.7 | Mon | 11:15–11:45 | EW 015 | **Strong light-matter interaction probed by cathodoluminescence spectroscopy** — •Fatemeh Chahshouri, Nahid Talebi |
| HL 3.1 | Mon | 9:30–10:00 | EW 202 | **Unraveling spin dynamics from charge fluctuations** — Eric Kleinherbers, •Jürgen König |
| HL 4.7 | Mon | 11:15–11:45 | EW 203 | **Influence of the Organic Cation Orientation on the Absorption Spectra of 2D Hybrid Organic-Inorganic Perovskites** — •Svenja Janke |
| HL 11.7 | Mon | 16:45–17:15 | EW 203 | **Strategic wafer-scale creation of telecom single-photon emitters in silicon for large-scale quantum photonic integrated circuits** — •Yonder Berencen |
| HL 20.1 | Tue | 9:30–10:00 | EW 203 | **Coherent ultrafast exciton dynamics mediated by vibronic couplings** — •Antonietta De Sio |
| HL 20.2 | Tue | 10:00–10:30 | EW 203 | **Merging electron microscopy with advanced photonics** — •Armin Feist, Guanhao Huang, Germaine Arend, Yujia Yang, Jan-Wilke Henke, Arslan Sajid Raja, F. Jasmin Kappert, Rui Ning Wang, Hugo Lourenço-Martins, Qiu Zheru, Junqiu Liu, Ofer Kfir, Tobias J. Kippenberg, Claus Ropers |
| HL 20.3 | Tue | 10:30–11:00 | EW 203 | **Nanotextured Surfaces Based on DNA** — •Irina Martynenko, Tim Liedl |
| HL 20.4 | Tue | 11:15–11:45 | EW 203 | **Advances in Quantum Light Generation for Quantum Communication** — •Tobias Heindel |
| HL 20.5 | Tue | 11:45–12:15 | EW 203 | **Membrane external-cavity surface-emitting lasers: A review at the first decade of research** — •Hermann Kahle |
| HL 28.1 | Wed | 9:30–10:00 | EW 203 | **Green-Kubo lattice dynamics approach to thermal transport in strongly anharmonic materials** — •Ivana Savić |
| HL 28.2 | Wed | 10:00–10:30 | EW 203 | **Hybrid crystal-glass heat conduction and radiative effects in disordered solids** — •Michele Simoncelli |
| HL 28.3 | Wed | 10:30–11:00 | EW 203 | **Engineering and probing phonons and thermal transport** — •Ilaria Zardo, Begoña Abad, Chaitanya Arya, Giulio de Vito, Yashpreet Kaur, Dominik M. Koch, Grazia Raciti, Aswathi K. Sivan, Jose M. Sojo, Johannes Trautvetter |
| HL 28.4 | Wed | 11:15–11:45 | EW 203 | **Challenges and opportunities of thermally anisotropic materials** — •Sebastian Reparaz |
| HL 29.1 | Wed | 9:30–10:00 | EW 561 | **Nonreciprocal charge transport on the edges of a quantum anomalous Hall insulator** — •Gertjan Lippertz, Anjana Uday, Andrea Bliesener, Lino Pereira, Alexey Taskin, Yoichi Ando |
| HL 40.7 | Thu | 11:15–11:45 | EW 201 | **Exciton transport in van der Waals antiferromagnet CrSBr** — •Florian Dirnberger, Sophia Terres, Akashdeep Kamra, Mikhail M. Glazov, Alexey Chernikov |
| HL 41.1 | Thu | 9:30–10:00 | EW 202 | **Quantum sensors and memories based on soft-clamped phononic membrane resonators** — •Albert Schliesser |

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| HL 41.2 | Thu | 10:00–10:30 | EW 202 | **Quantum mechanics-free subsystem with mechanical oscillators** — •Laure Mercier de Lepinay, Caspar Ockeloen-Korppi, Matthew Woolley, Mika Sillanpää |
| HL 41.3 | Thu | 10:30–11:00 | EW 202 | **Electrothermally tunable metal-graphene-siliconnitride membrane mechanical device** — •Elke Scheer, Mengqi Fu, Fan Yang |
| HL 41.4 | Thu | 11:15–11:45 | EW 202 | **From Nanomechanics to Spins** — •Christian Degen |
| HL 41.5 | Thu | 11:45–12:15 | EW 202 | **Enhanced cooling efficiency in nonlinear cavity optomechanics** — •Anja Metelmann, Nicolas Diaz-Naufal, David Zoepfl, Lukas Deeg, Christian Schneider, Mathieu Juan, Gerhard Kirchmaier |
| HL 45.1 | Thu | 14:00–14:30 | EW 203 | **Compact, plug-and-play module to generate high-quality photon states from quantum dots** — •Vikas Remesh |
| HL 49.1 | Thu | 15:00–15:30 | EW 561 | **Dynamical laser properties of tunnel-injection devices.** — •Michael Lorke, Frank Jahnke, Gadi Eisenstein, Johann-Peter Reithmeier |
| HL 53.7 | Fri | 11:15–11:45 | EW 201 | **Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene** — •Anna Seiler, Nils Jacobsen, Martin Statz, Fabian Geisenhof, Felix Winterer, Isabell Weimer, Tianyi Xu, Zhiyu Dong, Leonid Levitov, Fan Zhang, Thomas Weitz |
| HL 54.1 | Fri | 9:30–10:00 | EW 202 | **Tunneling spectroscopy of a phase-tunable topological insulator Josephson junction** — •Jakob Schluck, Ella N. Nikodem, Anton Montag, Alexander Ziesen, Mahasweta Bagchi, Zhiwei Wang, Fabian Hassler, Yoichi Ando |
| HL 54.2 | Fri | 10:00–10:30 | EW 202 | **Robust Majorana modes in topological material-based nanoelectronic hybrid devices** — •Kristof Moors |
| HL 54.3 | Fri | 10:30–11:00 | EW 202 | **Thermal and electric response of superconducting topological materials; are Majorana states more widespread than expected?** — •Ewelina Hankiewicz |
| HL 54.4 | Fri | 11:15–11:45 | EW 202 | **Tunable Josephson coupling in HgTe nanodevices** — •Martin P. Stehno |
| HL 54.5 | Fri | 11:45–12:15 | EW 202 | **Superconducting proximity effect in topological Dirac materials** — •Chuan Li, Anqi Wang, Caizhen Li, Chhunguang Chu, Zhimin Liao, Alexander Brinkman |
| HL 54.6 | Fri | 12:15–12:45 | EW 202 | **Exploring Josephson Junctions made of Topological Insulator Wires and Superconductors** — •Dieter Weiss |

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

See SYSD for the full program of the symposium.

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

## Invited Talks of the joint Symposium Advances in Ab-Initio Electronic Structure Theory of Time-Dependent and Non-Equilibrium Phenomena (SYES)

See SYES for the full program of the symposium.

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| SYES 1.1 | Tue | 9:30–10:00 | H 0105 | **Light control of charge transport and phase transitions** — •Sheng Meng |
| SYES 1.2 | Tue | 10:00–10:30 | H 0105 | **Probing the transport of the interacting electron-phonon system self-consistently and *ab initio*** — •Nakib Protik |
| SYES 1.3 | Tue | 10:30–11:00 | H 0105 | **In- and out-of-equilibrium ab initio theory of electrons and phonons** — •Gianluca Stefanucci |
| SYES 1.4 | Tue | 11:15–11:45 | H 0105 | **Phonon screening of excitons in semiconductors and insulators from first principles** — •Marina Rucsandra Filip |

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| SYES 1.5 | Tue | 11:45–12:15 | H 0105 | **Light-matter control of quantum materials: from Floquet to cavity engineering** — •Michael Sentef |

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

See SYEM for the full program of the symposium.

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| SYEM 1.1 | Wed | 9:30–10:00 | H 0105 | **Non-critical Materials Production for a Green Energy Transition** — •Anke Weidenkaff, Wenjie Xie, Marc Wiedenmeyer |
| SYEM 1.2 | Wed | 10:00–10:30 | H 0105 | **Strategies for the morphological design of photoactive oxynitride particles and electrodes for solar water-splitting.** — •Simone Pokrant |
| SYEM 1.3 | Wed | 10:30–11:00 | H 0105 | **Computational workflows for an accelerated design of novel materials and interfaces** — •Ivano Eligio Castelli |
| SYEM 1.4 | Wed | 11:30–11:45 | H 0105 | **Autonomous composition control of emerging nitride materials for solar energy conversion** — •Andriy Zakutayev |
| SYEM 1.5 | Wed | 11:45–12:00 | H 0105 | **Understanding and tailoring the catalytic activity of spinel and perovskite surfaces from first principles calculations** — •Rossitza Pentcheva |
| SYEM 1.6 | Wed | 12:00–12:15 | H 0105 | **Mastering Compositional Complexity in High Entropy Materials for Energy Applications - Towards Accelerated Materials Discovery by Integration of High-throughput Experimentation, Simulation, and Materials Informatics** — •Alfred Ludwig |

## Invited Talks of the joint Symposium Quantum Communication: Promises or Reality? (SYQC)

See SYQC for the full program of the symposium.

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| SYQC 1.1 | Fri | 9:30–10:00 | H 0105 | **Efficient Quantum Dot Micropillars for Quantum Networks** — David Dlaka, Petros Androvitsaneas, Andrew Young, Qirui Ma, Edmund Harbord, •Ruth Oulton |
| SYQC 1.2 | Fri | 10:00–10:30 | H 0105 | **Superconducting Single Photon Detectors - Limited only by the laws of physics** — •Andreas Fognini |
| SYQC 1.3 | Fri | 10:45–11:15 | H 0105 | **Laser triggering of quantum light sources using engineered optical pulses** — •Kimberley Hall |
| SYQC 1.4 | Fri | 11:15–11:45 | H 0105 | **Quantum Networks and Technologies** — •Rob Thew |

## Sessions

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|---|---|---|---|---|
| HL 1.1–1.12 | Mon | 9:30–13:00 | EW 015 | **Nitrides: Preparation and characterization I** |
| HL 2.1–2.13 | Mon | 9:30–13:00 | EW 201 | **2D Materials and Heterostructures: Photonic Aspects** |
| HL 3.1–3.11 | Mon | 9:30–12:45 | EW 202 | **Quantum Dots and Wires: Transport** |
| HL 4.1–4.12 | Mon | 9:30–13:00 | EW 203 | **Perovskite and Photovoltaics I (joint session HL/KFM)** |
| HL 5.1–5.8 | Mon | 9:30–11:45 | EW 561 | **Optical Properties I** |
| HL 6.1–6.10 | Mon | 9:30–12:45 | HFT-FT 131 | **Semiconductor Qubits (joint session QI/HL)** |
| HL 7.1–7.7 | Mon | 15:00–17:00 | ER 325 | **Transport properties I** |
| HL 8.1–8.11 | Mon | 15:00–18:00 | EW 015 | **Ultrafast Phenomena I** |
| HL 9.1–9.13 | Mon | 15:00–18:30 | EW 201 | **2D Materials and Heterostructures: Interlayer Excitons** |
| HL 10.1–10.11 | Mon | 15:00–18:00 | EW 202 | **Focus Session: Evolution of Topological Materials into Superconducting Nanodevices I (joint session HL/TT)** |
| HL 11.1–11.10 | Mon | 15:00–18:00 | EW 203 | **Materials and Devices for Quantum Technology I (joint session HL/QI)** |
| HL 12.1–12.7 | Mon | 15:00–16:45 | EW 561 | **Semiconductor Lasers I** |
| HL 13.1–13.60 | Mon | 15:00–18:00 | Poster E | **Poster I** |
| HL 14.1–14.28 | Mon | 15:00–18:00 | Poster F | **Poster II** |
| HL 15.1–15.6 | Mon | 16:45–18:15 | H 3007 | **Quantum Dots and Quantum Wires (joint session TT/HL)** |
| HL 16.1–16.8 | Tue | 9:30–11:45 | ER 325 | **Functional Semiconductors for Renewable Energy Solutions I** |
| HL 17.1–17.9 | Tue | 9:30–12:00 | EW 015 | **Organic Semiconductors** |

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| HL 18.1–18.13 | Tue | 9:30–13:00 | EW 201 | **2D Materials and Heterostructures: Emerging Materials and Phenomena** |
| HL 19.1–19.12 | Tue | 9:30–13:00 | EW 202 | **Quantum Dots and Wires: Optics I** |
| HL 20.1–20.5 | Tue | 9:30–12:15 | EW 203 | **Focus Session: Young Semiconductor Forum** |
| HL 21.1–21.8 | Tue | 9:30–11:45 | EW 561 | **Heterostructures, Interfaces and Surfaces I** |
| HL 22.1–22.20 | Tue | 11:00–15:30 | Poster F | **Focus Session: Young Semiconductor Forum** |
| HL 23.1–23.5 | Tue | 11:45–13:00 | H 3007 | **Focus Session: Nanomechanical Systems for Classical and Quantum Sensing I (joint session TT/DY/HL/QI)** |
| HL 24.1–24.7 | Wed | 9:30–11:15 | H 3007 | **Graphene and 2D Materials (joint session TT/HL)** |
| HL 25.1–25.11 | Wed | 9:30–12:45 | ER 325 | **Oxide Semiconductors I** |
| HL 26.1–26.10 | Wed | 9:30–12:15 | EW 201 | **2D Materials and Heterostructures: Quantum Emitters and Defects** |
| HL 27.1–27.7 | Wed | 9:30–11:30 | EW 202 | **Quantum Dots and Wires: Optics II** |
| HL 28.1–28.9 | Wed | 9:30–13:00 | EW 203 | **Focus Session: Heat transport at the nanoscale: theory meets experiment** |
| HL 29.1–29.8 | Wed | 9:30–12:00 | EW 561 | **Quantum Transport and Quantum Hall Effects** |
| HL 30.1–30.8 | Wed | 10:00–12:15 | EW 015 | **Ultrafast Phenomena II** |
| HL 31.1–31.5 | Wed | 11:45–13:00 | EW 202 | **Focus Session: Evolution of Topological Materials into Superconducting Nanodevices II (joint session HL/TT)** |
| HL 32.1–32.5 | Wed | 15:00–16:15 | EW 015 | **Spin Phenomena in Semiconductors** |
| HL 33.1–33.5 | Wed | 15:00–16:15 | EW 201 | **2D Materials and Heterostructures: Optoelectronics** |
| HL 34.1–34.10 | Wed | 15:00–17:45 | EW 202 | **Focus Session: Nanomechanical Systems for Classical and Quantum Sensing II (joint session HL/DY/TT/QI)** |
| HL 35.1–35.5 | Wed | 15:00–16:15 | EW 203 | **THz and MIR** |
| HL 36.1–36.60 | Wed | 18:00–20:30 | Poster E | **Poster III** |
| HL 37.1–37.29 | Wed | 18:00–20:30 | Poster F | **Poster IV** |
| HL 38.1–38.7 | Thu | 9:30–11:30 | ER 325 | **Oxide Semiconductors II** |
| HL 39.1–39.5 | Thu | 9:30–10:45 | EW 015 | **Outreach / Wissenschaftskommunikation** |
| HL 40.1–40.12 | Thu | 9:30–13:00 | EW 201 | **2D Materials and Heterostructures: Magnetic Properties** |
| HL 41.1–41.8 | Thu | 9:30–13:00 | EW 202 | **Focus Session: Nanomechanical Systems for Classical and Quantum Sensing III (joint session HL/DY/TT/QI)** |
| HL 42.1–42.14 | Thu | 9:30–13:15 | EW 203 | **Perovskite and Photovoltaics II (joint session HL/KFM)** |
| HL 43.1–43.8 | Thu | 9:30–11:45 | EW 561 | **Optical Properties II** |
| HL 44.1–44.11 | Thu | 14:00–17:00 | EW 015 | **Nitrides: Preparation and characterization II** |
| HL 45.1–45.9 | Thu | 14:00–16:45 | EW 203 | **Materials and Devices for Quantum Technology II (joint session HL/QI)** |
| HL 46.1–46.7 | Thu | 15:00–17:00 | ER 325 | **Transport properties II** |
| HL 47.1–47.8 | Thu | 15:00–17:00 | EW 201 | **2D Materials: Heterostuctures** |
| HL 48.1–48.6 | Thu | 15:00–16:30 | EW 202 | **Quantum Dots and Wires: Growth** |
| HL 49.1–49.6 | Thu | 15:00–16:45 | EW 561 | **Semiconductor Lasers II** |
| HL 50 | Thu | 17:00–18:30 | EW 202 | **Members' Assembly** |
| HL 51.1–51.6 | Fri | 9:30–11:00 | ER 325 | **Functional Semiconductors for Renewable Energy Solutions II** |
| HL 52.1–52.9 | Fri | 9:30–12:00 | EW 015 | **Nitrides: Devices** |
| HL 53.1–53.9 | Fri | 9:30–12:15 | EW 201 | **2D Materials and Heterostructures: (Twisted) Bilayers (joint session HL/TT)** |
| HL 54.1–54.6 | Fri | 9:30–12:45 | EW 202 | **Focus Session: Evolution of Topological Materials into Superconducting Nanodevices III (joint session HL/TT)** |
| HL 55.1–55.13 | Fri | 9:30–13:00 | EW 203 | **Perovskite and Photovoltaics III (joint session HL/KFM)** |
| HL 56.1–56.6 | Fri | 9:30–11:00 | EW 561 | **Heterostructures, Interfaces and Surfaces II** |

## Members' Assembly of the Semiconductor Physics Division

Thursday 17:00–18:30 EW 202

- Bericht
- Junges Halbleiter-Forum / Young Semiconductor Forum
- Verleihung des Posterpreises
- Verschiedenes

# HL 1: Nitrides: Preparation and characterization I

Time: Monday 9:30–13:00 Location: EW 015

HL 1.1 Mon 9:30 EW 015

**Time-resolved ellipsometry on degenerately doped cubic GaN** — •Elias Baron[1], Rüdiger Goldhahn[1], Michael Deppe[2], Donat J. As[2], Shirly Espinoza[3], Martin Zahradník[3], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany — [3]ELI Beamlines, ELI ERIC, Dolní Břežany, Czech Republic

The interest in ultra-fast processes in semiconductors has steadily increased in recent years, as modern technologies require faster and faster electronics and optics. Highly sensitive measurement techniques are essential for researching these phenomenons. In this context, time-resolved spectroscopic ellipsometry (TRSE) proved to be an excellent technique for determining the transient optical properties. Additionally, the metastable cubic phase of the well-known GaN offers advantageous properties for investigating fundamental processes in excited semiconductors. We present our analysis of thin film cubic GaN, deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation and doped by either Ge or Si up to $9\times10^{19}\,\mathrm{cm}^{-3}$. TRSE measurements, based on a pump-probe approach in the UV spectral range are performed using a 266 nm pump-beam. The electron-hole pairs generated by this pump-beam influence the optical properties due to many-body effects like band gap renormalization and Burstein-Moss shift. The impact of these effects vary depending on the doping concentration. Furthermore, a free-carrier profile from top to bottom has to be considered for an accurate description.

HL 1.2 Mon 9:45 EW 015

**Optical properties of cubic $In_xGa_{1-x}N$ thin films** — •Jonas Rose[1], Elias Baron[1], Rüdiger Goldhahn[1], Mario Zscherp[2], Silas A. Jentsch[2], Sangam Chatterjee[2], Jörg Schörmann[2], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Cubic InGaN (c-InGaN) is a promising material for fabricating highly efficient optoelectronical devices and can potentially replace its hexagonal counterpart for certain applications. Due to the lack of internal polarization fields and lower band gap energies c-InGaN is a suitable candidate for applications in the visible spectrum. Especially InGaN/GaN quantum wells can be used for green light-emitting devices. Therefore, the knowledge of its optical properties is of special interest. In this context, spectroscopic ellipsometry is a sophisticated experimental technique due to its high sensitivity as well as contact- and destruction-free operation. Recently, several breakthroughs in crystal growth regarding structural quality and range of In-content have been achieved.

We present our investigation of c-InGaN thin films deposited by plasma-assisted molecular beam epitaxy (MBE) on 3C-SiC/Si substrates in (001) orientation. Spectroscopic ellipsometry measurements in the IR and VIS-UV spectral range yield the dielectric function containing phonon and plasmon contributions as well as interband transitions. Additionally, many-body effects affecting the absorption edge are taken into account.

HL 1.3 Mon 10:00 EW 015

**Time-resolved cathodoluminescence spectroscopy of oxygen related defects in AlN layers** — •Barbara Szafranski, Lukas Peters, Andreas Waag, and Tobias Voss — Institute of Semiconductor Technology, Braunschweig University of Technology, Germany

High temperature annealing (HTA) of sputtered AlN leads to a substantial improvement of the crystal quality. However, during the annealing process, a large number of point defects like oxygen is introduced. Oxygen has a double-edged role during HTA.

We therefore analyzed oxygen defects in AlN layers with cathodoluminescence (CL) spectroscopy. The 350 nm thick AlN layers were treated with HTA at different temperatures. The process has been optimised to lead to very high crystal quality.

At room temperature, CL spectroscopy shows a broad (FWHM 650 meV) luminescence band centered at about 3.66 eV (340 nm), which we correlate with oxygen point defects. To study the charge carrier dynamics of these defects in AlN, time-resolved CL measurements have been performed. The defect related emission is characterized by a complex multiexponential decay with a fast component of about 1 ns and a slow component of tens to hundreds of nanoseconds. In agreement with Genji et al., we attribute the short decay time to the radiative transition from the conduction band-edge states to $(V_{Al}-2O_N)^{1-}$ and $(V_{Al}-O_N)^{2-}$ and the long decay times to trapping and detrapping processes of the charge carriers via shallow traps [1].

[1] Kumihiro Genji and Takashi Uchino, Appl. Phys. Lett. 109, 021113 (2016).

HL 1.4 Mon 10:15 EW 015

**n-type doping of GaN via pulsed sputter epitaxy** — •Florian Hörich, Jürgen Bläsing, Jona Grümbel, Martin Feneberg, Rüdiger Goldhahn, Armin Dadgar, and André Strittmatter — Otto-von-Guericke University

Semiconductor devices like HEMTs typically employ a highly insulating buffer and a current transport layer. Recent developments in reactive sputter epitaxy have led to high resistances and breakdown field strenghs for GaN /1/. This talk focusses on n-type doping of GaN via co-sputtering with Si and Ge. For both dopants carrier concentrations ranging from $10^{17}$ up to $10^{20}$ $cm^{-3}$ are feasible. The carrier density evaluated by Hall-effect and by PL measurements, evaluated for the free-carrier concentration by the bandgap shift (Burstein-Moss effect) /2/, are in good agreement. Just like MOVPE grown layers, highly Si doped layers tend to surface roughening due to SiN formation. This effect is even more pronounced for Ge doped layers. The relatively low growth temperature of 750 °C likely promotes $Ge_xN_y$ formation. Contrary to MOVPE results, XRD measurements show an additional peak in the $\theta/2\theta$-Scan for Ge doped layers, indicating a distortion of the lattice.

/1/ A. Dadgar et al, Phys. Stat. Sol. a 220, 2200609 (2022) /2/ M. Feneberg et al. Physical Review B 90, 075203397 (2014)

HL 1.5 Mon 10:30 EW 015

**Bandgap Engineering in Cubic Nitrides: a Theoretical Study** — •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

For new applications like integrated RGB LEDs, a precise bandgap engineering over the full visible spectrum is desired. This can be achieved by alloying a narrow bandgap material such as indium nitride (InN) or scandium nitride (ScN) with a wide bandgap semiconductor such as gallium nitride (GaN) or aluminum nitride (AlN).

These material systems like (Al,Sc)N or (In,Ga)N are random alloys that require specific techniques such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2] to ensure accurate calculations. To properly predict the fundamental electronic band gap, we use the low computational cost LDA-1/2 method [3]. In this study, we present our results on structural and electronic properties such as stability, lattice parameter, band gap and phonon modes.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). https://doi.org/10.1103/PhysRevB.88.094421

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. 65, 353 (1990). https://doi.org/10.1103/PhysRevLett.65.353

[3] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). https://doi.org/10.1103/PhysRevB.78.125116

HL 1.6 Mon 10:45 EW 015

**deciphering the origin of small pits in GaInN/GaN quantum wells structures: correlation of defect formation and growth conditions** — •Mahdi Khalili Heyarjaribi[1,2], Rodrigo de Vasconcellos Lourenço[1,2], Uwe Rossow[1,2], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

Threading dislocations are non-radiative centers and can affect the luminescence efficiency of light emitters based on GaInN/GaN quantum wells (QWs).Specially for heteroepitaxial growth,i.e on sapphire substrate, the dislocation density is high, leading to a significantly reduced

luminescence efficiency. This issue can be addressed by intentionally creating V-pits, screening the threading dislocations cores. We have observed that sometimes additional pits are visible after the growth of the quantum well stack. Those pits are far smaller in size and usually appear as pairs, and may be associated to defects, e.g. stacking faults, which are formed during QW growth and may act as non-radiative centers. Employing scanning electron microscope (SEM) imagery, we investigate the V-pits. The analysis of thousands of images is a very time consuming and laborious procedure. We developed a model, using YOLO machine learning algorithm, which can objectively characterize the pits,their size distribution, density, and can selectively focus on the small pits.The trained model is more efficient and faster than conventional methods.Using the results and systematic variations of structural parameters, we elucidate the origin of the small pits.

**15 min. break**

**Invited Talk** HL 1.7 Mon 11:15 EW 015

**Strong light-matter interaction probed by cathodoluminescence spectroscopy** — •Fatemeh Chahshouri[1] and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel, Nano, Surface, and Interface Science -KiNSIS, Kiel University, 24098 Kiel, Germany

Electron microscopy is a powerful tool that offers detailed views of a composition of biological, chemical, and semiconductor structures with atomic-scale resolution. Additionally, it enables us to study quantum phenomena at the nanoscale and explore exciting phenomena, such as probing (quantum-)optical excitation and tailoring the shape of electron beams, where the latter further allows for more advanced characterization techniques. In this talk, we will discuss the functionality of cathodoluminescence spectroscopy in investigating the formation and propagation of exciton-polaritons in van der Waals materials. We will further discuss how generated secondary electron carriers in the heterostructure of group III nitride materials can interact with defects and Schottky barriers and generated two-dimensional electron gas inside the heterojunction. Furthermore, we will describe our numerical investigations on modulating and shaping the electron wavepacket after interacting with laser-induced optical near-fields in the vicinity of the material. Our work introduces new possibilities, allowing electrons to be utilized as a nanoscale source for probing matter and opens up avenues for improving state-of-the-art electron microscopy through the use of tunable electron beams in enhancing the electron beam interaction with light and matter.

HL 1.8 Mon 11:45 EW 015

**HAXPES Study of $Al_{1-x}Sc_xN$-based Ferroelectric Capacitors** — •Oliver Rehm[1], Lutz Baumgarten[2], Roberto Guido[3], Pia Düring[1], Andrei Gloskovskii[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[1] — [1]Uni Konstanz, Konstanz, Germany — [2]FZJ, Jülich, Germany — [3]NaMLab, Dresden, Germany — [4]DESY, Hamburg, Germany — [5]TU Dresden, Dresden, Germany

The novel ferroelectric (FE) material $Al_{1-x}Sc_xN$ exhibits a large remanent polarization and coercive field, with huge potential for the next generation of nonvolatile memory devices. However, the application of AlScN-based thin films as active FE is currently hampered by cycling endurance and leakage issues, which are worse than that of $HfO_2$.

The present work focuses on exploring the chemical properties of $Al_{0.83}Sc_{0.17}N$ thin films (60 nm) using hard x-ray photoelectron spectroscopy (HAXPES). Studying both W-capped and uncapped samples, we show that AlScN is not stable in air due to surface-enhanced oxidation over long periods (weeks to months). By comparing the contribution of Sc and Al relative to the overall oxidation of $Al_{1-x}Sc_xN$, we assume that oxygen tends to occupy a neighbour lattice site of Sc, resulting in an enhanced oxidation of Sc compared to Al. Moreover, the oxidation process causes N atoms to be removed from their lattice sites, likely leading to an incorporation of interstitial N, which is deduced from the observation of a surface-enhanced spectral feature of the N 1s core-level.

O. Rehm, L. Baumgarten, M. Müller et al., in preparation

HL 1.9 Mon 12:00 EW 015

**Multiphonon Raman scattering in rocksalt ScN** — •Stefan Wolf[1], Jona Grümbel[1], Yuichi Oshima[2], Christopher Lüttich[1], Florian Hörich[1], Armin Dadgar[1], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität, Universitätsplatz 2, 39106, Magdeburg — [2]Research Center for Electronic and Optical Materials, National Institute for Materials Science , 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

We investigate rocksalt ScN films with different free carrier concentration using Raman spectroscopy. Two different sets of samples were used for our measurements: (I) ca. 300nm thick ScN grown by sputter epitaxy and (II) 0.4 $\mu m$ up to 40 $\mu m$ thick ScN grown by HVPE. The HVPE grown ScN exhibits a very good crystalline structure, with carrier concentration varying between $10^{18}cm^{-3}$ and $10^{20}cm^{-3}$, while for ScN grown by sputter epitaxy, the carrier concentrations even reach $10^{21}cm^{-3}$ or more. We obtain detailed information about the impact of free carriers on coupled optical phonon-plasmon (LPP) modes up to a scattering order of $n_{LPP} = 3$.

The observed frequency shift of the first and second order LPP modes with respect to the carrier concentration shows an overdamped behaviour, indicating strong electron-electron interaction. As expected, transverse optical phonon modes show no significant frequency shift over the whole carrier concentration range. Correct assignment of multiphonon lines and possible future steps in understanding their behaviour will be discussed.

HL 1.10 Mon 12:15 EW 015

**Point defect diffusion in GaInN/GaN quantum well structures** — •Rodrigo De Vasconcellos Lourenco, Philipp Henning, Philipp Horenburg, Uwe Rossow, Heiko Bremers, and Andreas Hangleiter — Institute of Applied Physics, Technische Universität Braunschweig, Germany

A reduction of the point defect density in light-emitters based on GaInN/GaN quantum wells (QW) is desired for maximising the internal quantum efficiency. We investigate the non-radiative lifetime of GaInN/GaN single QWs grown on In-free and In-containing underlayers (UL). The non-radiative lifetime of SQWs increases with UL thickness in both cases. Since the non-radiative lifetime is inversely proportional to the defect density and as V-pits efficiently suppress the recombination at threading dislocations, our result suggests a point defect density profile over distance between the high temperature GaN buffer layer and the QW. Hence, a simple solution to the diffusion equation allows to accurately fit our data and yields a defect diffusion coefficient. point defect diffusion is a thermally activated process, associated with a defect migration barrier, which is in the range expected for the nitrogen vacancy in n-type GaN. Surprisingly, an attempt to reproduce the results lead to non-radiative lifetimes about one order of magnitude lower than previously, but with the same activation energy. This means that diffusion is prevalent in the same way, but with a different boundary condition, i.e. a higher density of point defects in the underlying GaN buffer.

HL 1.11 Mon 12:30 EW 015

**Phases of sputtered $Hf_xN_y$: XRD, Ellipsometry and Raman spectroscopy studies** — •Jona Grümbel, Christopher Lüttich, Jürgen Bläsing, Armin Dadgar, Martin Feneberg, and Rüdiger Goldhahn — Otto-von-Guericke-Universität, Universitätsplatz 2, 39106, Magdeburg,

Several phases of the binary material system $Hf_xN_y$ are predicted to be stable or metastable, where the thermodynamically preferred rocksalt ($Fm\bar{3}m$) structured HfN exhibits the lowest formation energy and a metallic character. The metastable modified zincblende like ($I4\bar{3}d$) structured $Hf_3N_4$ is predicted to be semiconducting. Aiming for metallic rs-HfN, various samples were prepared via DC magnetron sputtering under varying conditions, e.g. using $N_2$ or $N_2$+$NH_3$ as sputter gases. Surprisingly, samples with high ammonia flow (>10 sccm) lose their golden metallic color but exhibit typical thin film interference colors, indicating transparency in the visible spectral range. We apply UV ellipsometry and Raman spectroscopy measurements to proof, that $Hf_xN_y$ grown with increasing ammonia flux becomes semiconducting with an absoprtion edge of ≈ 3 eV. Annealing metallic HfN samples under ammonia atmosphere yields the same semiconductiong $Hf_xN_y$ phase with several narow Raman bands and an absorption edge of ≈ 3 eV as well. Surprisingly, XRD powder diffraction indicates a new phase only for the annealed sample. Detailed analysis of the optical characteristics will be presented as well as a comparison to various theroretical calculations of different $Hf_xN_y$ phases.

HL 1.12 Mon 12:45 EW 015

**Highly resolved cathodoluminescence spectra of N-polar homoepitaxial AlN** — •Domenik Spallek[1], Gwénolé Jacopin[2], Len van Deurzen[3], Jashan Singhal[3], Jimy Encomendero[3], Oliver Brandt[1], Debdeep Jena[3], and Jonas Lähnemann[3] —

[1]Paul-Drude-Institut, Berlin, Germany — [2]Institute Néel, CNRS, Grenoble, France — [3]Cornell University, Ithaca, New York, USA

As a semiconductor with an ultra-wide band gap, AlN is an interesting material for applications in optoelectronic devices such as UV-LEDs. Additionally, its high thermal conductivity and breakdown field are advantageous for applications in high power electronics. High quality AlN layers of either Al or N polarity can be grown homoepitaxially on commercial substrates by molecular beam epitaxy (MBE) [1]. Besides serving as potential basis for device structures, the low point defect and dislocation densities result in high luminous efficiencies, which makes such layers a suitable platform for comprehensive investigation of their fundamental excitonic emission.

We focus on an N-polar AlN layer and present near-band-edge cathodoluminescence spectra as a function of temperature, as well as for different measurement geometries. An improved spectral resolution uncovers additional emission lines compared with Ref. 1. The various emission lines can be assigned to free excitons with different symmetries and defect-bound states of different origin, as well as their phonon replicas. Thus, this study contributes to the resolution of controversies in the attribution of excitonic emission lines in AlN.

[1] van Deurzen *et al.*, APL Mater. **11**, 081109 (2023)

## HL 2: 2D Materials and Heterostructures: Photonic Aspects

Time: Monday 9:30–13:00 Location: EW 201

HL 2.1 Mon 9:30 EW 201

**Measuring the complex valley polarization nonlinear susceptibility in monolayer $WSe_2$** — •Paul Herrmann, Sebastian Klimmer, Till Weickhardt, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany

Valleytronics suffers from the lack of an ideal method to probe the valley degree of freedom. Both state of the art methods, namely polarized photoluminescence and Kerr rotation, are insensitive to the complex nature of valley polarization (VP). More generally, one can view measuring VP as probing broken time-reversal (TR) symmetry. As second harmonic generation (SHG) is sensitive to symmetry, it was proposed as a probe of VP. However, said method of probing the rotation in the SHG pattern of elliptically polarized pulses [1] suffers from limited valley adressability and also disregards the complex nature of VP. In this work we overcome both aforementioned problems [2]. We develop and demonstrate a new method that probes the interference between electric-dipole and VP in the SHG signal when we directly excite at ±K resonance with circularly polarized light. We show that such interference can only be explained by taking into consideration the complex nature of VP, in analogy to the magnetic- to electric-dipole interference observed in bulk magnets [3]. Our work provides a new method for detection of VP and we argue that it could be extended to probe broken TR symmetry in other crystal classes.

[1] Herrmann, P. et al.: small 2023 19:2301126
[2] Herrmann, P. et al.: arXiv 2023 2310.16549
[3] Fiebig, M. et al.: PRL 1994 15(73)

HL 2.2 Mon 9:45 EW 201

**Theory of in-plane magnetic field dependence of excitonic spectra in atomically thin semiconductors** — •Michiel Snoeken, Andreas Knorr, and Henry Mittenzwey — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The linear absorption spectrum of TMDC monolayers under the influence of an in-plane magnetic field is studied by developing a microscopic theory in an excitonic picture. It is shown that in-plane magnetic fields induce coupling between spin-bright and spin-dark exciton transitions, resulting in the brightening of spin-dark excitons in the linear spectrum with increasing in-plane field-strength. Numerical evaluation shows that the energy splitting of these excitonic states increases with field strength and the relative intensities of the $A_{1s}$ and $Ad_{1s}$ converge to saturation after an initial quadratic growth. Some analytical limit cases are discussed.

HL 2.3 Mon 10:00 EW 201

**Symmetry and handedness of chiral tellurium under polarized Raman spectroscopy** — •Davide Spirito[1], Sergio Marras[2], and Beatriz Martín García[3,4] — [1]IHP-Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Istituto Italiano di Tecnologia - Materials Characterization Facility, Genova 16163, Italy — [3]CIC nanoGUNE BRTA, 20018 Donostia-San Sebastián, Basque Country, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain

Trigonal tellurium is a model low-dimensional material for the study of electrons and phonons in chiral systems. Here we show how the response of tellurium to polarized light depends on the crystal orientation, which has implication for optical properties and electron transport studies. By linearly polarized Raman spectroscopy we identify different crystal faces and the orientation of the trigonal axis, based on typical patterns derived from the analysis of the symmetry of the crystal. Furthermore, by circularly polarized measurements we determine the handedness only for incidence parallel to the trigonal axis, with the observation of different peaks shift for left- and right-handed crystals. We support our findings with X-ray diffraction and chirality-sensitive chemical etching, providing a robust insight for the analysis chiral and low-dimensional materials.

HL 2.4 Mon 10:15 EW 201

**Interaction of 2D materials with laser-written waveguide circuits** — •Alina Schubert[1], Karo Becker[1], Marco Kirsch[1], Jakob Kuhlke[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Matthias Heinrich[1], and Tobias Korn[1] — [1]Institut für Physik, Universität Rostock, 18059 Rostock, Germany — [2]Ferdinand Braun Institut, Leibnitz Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

The remarkable optical properties of monolayer transition metal dichalcogenides (TMDCs) are determined by strongly bound excitons. Currently, most of the micro-photoluminescence measurements are performed with light polarized in the plane of the TMDC layer. However, so-called dark excitons that emit z-polarized light propagating along the TMDC layer require detection from the side [1, 2].

Our intention is to probe TMDCs in this direction by depositing them onto a fused silica glass substrate containing femtosecond laser direct written waveguides [3]. By defining the waveguide near the surface of the glass, interactions of the waveguide's evanescent field and the TMDC are enabled.

Our micro-photoluminescence setup that couples into the waveguides and simultaneously detects light perpendicular to the TMDC layer has the potential to excite and detect the x,y and z polarization of the PL signal, allowing for direct observations of dark excitons.

[1] X.-X. Zhang et al., Phys. Rev. Lett., 115 (2015).
[2] G. Wang et al., Phys. Rev. Lett., 119 (2017).
[3] A. Szameit et al., J. Phys. B.: At. Mol. Opt. Phys., 43 (2010).

HL 2.5 Mon 10:30 EW 201

**Simulation of waveguide-coupled graphene-based double-layer straight and ring modulator** — •Pawan Kumar Dubey[1], Ashraful Islam Raju[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP- Leibniz Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

On-chip integrated, graphene-based optical modulators are state-of-the-art optoelectronics devices with numerous applications in emerging photonics technologies, providing the advantages of high modulation efficiency, high broadband application and low power consumption. Liu et al.2012 experimentally demonstrated a double-layered straight modulator with a modulation depth of just 0.16 dB/$\mu$m for the first time. This design had miniscule waveguide light interaction with the graphene layer, resulting in low modulation efficiency. A novel method emerged to elevate this interaction further, where the graphene layer was integrated with silicon nitride-based ring resonators. Taking this approach as a reference, we present an FDTD simulation of double-layer graphene-based ring modulators. We have studied the design parameters of the ring modulator, such as the radius, shape of the resonator, and graphene area, that affect the modulation efficiency. We have optimised the design of the ring resonator working near the

critical coupling condition, achieving a modulation depth of 3.5 dB/V, which is 20 times better than our previously simulated double-layer straight modulator design.

HL 2.6 Mon 10:45 EW 201

**Second-order temporal coherence of polariton lasers based on an atomically thin crystal in a microcavity** — •Hangyong Shan[1], Jens-Christian Drawer[1], Meng Sun[2], Carlos Anton-Solanas[5], Martin Esmann[1], Kentaro Yumigeta[6], Sefaattin Tongay[6], Sven Höfling[4], Ivan Savenko[3], and Christian Schneider[1] — [1]Oldenburg University, Oldenburg, Germany — [2]Beijing University of Technology, Beijing, China — [3]Guangdong Technion Israel Institute of Technology, Shantou, China — [4]Würzburg University, Würzburg, Germany — [5]Universidad Autónoma de Madrid, Madrid, Spain — [6]Arizona State University, Arizona, USA

Bosonic condensation and lasing of exciton-polaritons in microcavities is a fascinating solid-state phenomenon. Here, we study the photon statistics via the second-order temporal coherence of polariton lasing emerging from an optical microcavity integrated with an atomically thin MoSe2 crystal. In our experiments, we observe distinct polariton dispersions and characteristic features of bosonic lasing. With the utility of Hanbury Brown and Twiss (HBT) setup, we investigate macroscopic polariton phase transition for varying excitation powers and temperatures. The lower-polariton exhibits photon bunching below the threshold, implying a dominant thermal distribution of the emission, while above the threshold, the second-order correlation transits towards unity, which evidences the formation of a coherent state. Our findings are in agreement with a microscopic numerical model based on the Lindblad master equation, which explicitly includes scattering with phonons on the quantum level.

**15 min. break**

HL 2.7 Mon 11:15 EW 201

**Magnification of Plasmon Resonances in Monolayer MoS2 via Conjugated Molecular Adsorbates** — Juan Pablo Guerrero-Felipe[1], •Ana M. Valencia[2,3], and Caterina Cocchi[2,3] — [1]Department of Physics, Freie Universität Berlin — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [3]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin

The adsorption of carbon-conjugated molecules represents an established route to tune the electronic and optical properties of transition metal dichalcogenide (TMDC) monolayers. Here, we demonstrate from the first principles such a functionalization with prototypical compounds pyrene and tetracene enhance the magnitude of selected plasmon resonances in the MoS2 layer, without significantly altering their energy and dispersion. Our results indicate that such a magnification can be achieved by proper alignment of the molecules concerning the direction of the transferred momentum. The distinct signatures in the loss function of the interface compared to those of its constituents suggest not only the presence of non-negligible interactions between them but also the possibility of using electron energy loss spectroscopy to detect the presence and the orientation of molecular adsorbates on TMDCs. J.P. Guerrero-Felipe, et al., arXiv:2311.17613 [cond-mat.mtrl-sci]

HL 2.8 Mon 11:30 EW 201

**Coupling of excitons in few-layer WS2 films with a hybrid plasmon polariton at room temperature** — •Yuhao Zhang[1], Hans-Joachim Schill[1,2], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, 53115 Bonn, Germany — [2]Electron Microscopy and Analytics, Center of Advanced European Studies and Research (caesar), 53175 Bonn, Germany

Composite structures formed by the combination of plasmonics nanostructures that tightly confine light and TMDC thin film with a strong exciton resonance offer unique capabilities to investigate and engineer light-matter interactions in solid-state systems. So far, most research has focused on the strong coupling between plasmonic structures and TMDC monolayers. The strong coupling between few-layer TMDC with extended plasmonic nanostructures is still a largely unexploited territory.

In this work, we report on the room-temperature interaction of few layer WS2 thin films (monolayer to qudrilayer) with a tapered nanograting structure milled into a monocrystalline silver flake. The bare nanograting structure features hybrid plasmon polaritons (HPP) with three polariton branches. When a WS2 monolayer is deposited on the nanogroove array with an optimized design, the reflection spectra show an avoided crossing of the exciton mode and the lower plasmon polariton branch with a Rabi splitting of 68 meV indicating strong exciton-plasmon polariton coupling. The Rabi splitting increases to more than 100 meV in the case of the quadrilayer.

HL 2.9 Mon 11:45 EW 201

**Spectrally and topologically tunable polaritons based on two-dimensional crystals in a photonic lattice** — Lukas Lackner[1], Christoph Bennenhei[1], Oleg Egorov[2], Anthony Enzerhof[1], Victor Mitryakhin[1], Falk Eilenberger[2], Sefaattin Tongay[3], •Martin Esmann[1], and Christian Schneider[1] — [1]Carl von Ossietzky University, Oldenburg, Germany — [2]Friedrich Schiller University, Jena, Germany — [3]Arizona State University, Tempe, Arizona, USA

Engineering hybrid light-matter states in tailored photonic lattices is a key asset for the emulation of topological Hamiltonians interlinking fundamental aspects of photonics, information processing and solid state physics. Room temperature-stable excitons in atomically thin crystals are an ideal active medium for this purpose, since they couple strongly to light and bear the potential to harness giant non-linearities. Here, we study spectrally tunable exciton-polaritons of a WS2 monolayer in a high quality open cavity at room temperature [1]. We imprint a photonic lattice into the cavity, which emulates the canonical Su-Schrieffer-Heeger (SSH) Hamiltonian [2] and generate a topological mode at a domain boundary between two lattices characterized by different topological invariants. Our optical experiments reveal a spectral tunability of the topologically protected mode over a range as large as 80 meV. Utilizing the unique tilt-tunability of our implementation, we transform the SSH-lattice into a Stark-ladder and fundamentally change its topological class.

[1] L. Lackner et al., Nat Commun 12, 4933 (2021)
[2] W. P. Su et al. PRL 42, 1698 (1979)

HL 2.10 Mon 12:00 EW 201

**2D Semiconductor-Plasmonic Hybrids: Strong Coupling, Exciton Localization, and Single Photon Emission** — •Lara Greten, Robert Salzwedel, Malte Selig, and Andreas Knorr — Nichtlineare Optik und Quantenelektronik, Institut für Theoretische Physik, Technische Universität Berlin, Germany

Monolayers of transition metal dichalcogenides (TMDCs) display strong light-matter interaction dominated by tightly bound excitons. In contrast, metal nanostructures support localized plasmons, allowing for nanoscale electric field control. This talk is focused on a microscopic description of the interplay between excitons and plasmons, combining Maxwell's and excitonic Bloch equations [1,2,3]. The theory is applied to three situations: (a) exciton localization within plasmon-induced near-field potentials [2], (b) exciton-plasmon strong coupling in 2D lattices with a spectral splitting of 100 meV [3], and (c) Purcell-enhanced single-photon generation [4].

[1] L. Greten, R. Salzwedel et al., physica status solidi (a) 2300102 (2023)
[2] R. Salzwedel, L. Greten et al., arXiv:2305.11099 (2023)
[3] L. Greten, R. Salzwedel et al., arXiv:2309.09673 (2023)
[4] M. von Helversen, L. Greten et al., 2D Mater. 10 045034 (2023)

HL 2.11 Mon 12:15 EW 201

**Light-matter interaction of TMDCs in an open cavity** — •Shiyu Huang[1], Edith Wietek[2], Johannes Düreth[1], Simon Betzold[1], Monika Emmerling[1], Takashi Taniguchi[3], Kenji Watanabe[3], Sven Höfling[1], Alexey Chernikov[2], and Sebastian Klembt[1] — [1]Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg, Deutschland — [2]Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Excitons in monolayer transition metal dichalcogenides (TMDCs) and their heterostructures can strongly couple to electromagnetic fields, and monolayer $WS_2$ is a fascinating medium for studying hybrid light-matter states at room temperature. We report the monolayer $WS_2$ encapsulated in hBN employed in an open cavity, where two distributed Bragg reflectors were utilized to strongly confine the photonic field. When reducing the cavity length and thus the number of cavity modes, we reach the strong coupling regime of light-matter interaction at room

temperature. Structured cavity mirrors are employed to study polariton physics and has potential to investigate exciton-polariton interactions. Furthermore, the open cavity approach paves the way to integration of $WS_2/WSe_2$ heterostructure with Moiré supperlattices in high-Q microcavities, which is promising to study exciton topology.

HL 2.12 Mon 12:30 EW 201

**Tunable All-Graphene Metasurfaces Based on Bound States in the Continuum** — •Michael Hirler, Thomas Weber, Jonas Biechteler, and Andreas Tittl — Chair in Hybrid Nanosystems, Ludwig-Maximilians-University Munich, Germany

We present an all-graphene optical metasurface based on Bound States in the Continuum (BICs). While graphene excels with tunable, long-lived plasmons with outstanding near-field confinement in the mid-infrared, the physics of BICs allows for the generation of spectrally narrow resonances with precise control over the radiative loss channel. This can be achieved by means of patterning monolayer graphene at subwavelength dimensions in various asymmetric structures. Furthermore, the incorporation of a bottom gate separated by an insulating layer allows for electric gating and, thus, the post-fabrication tuning of the plasmonic response. In particular, leveraging the tunability via asymmetric gating opens a new gateway for dynamic control of light-matter-interaction. On the basis of numerical simulations, we discuss the potential and limits of these metasurfaces, while progresses and challenges in realizing a first prototype via electron beam lithography are also outlined. Our metasurface constitutes a promising platform for compact, affordable point-of-care applications such as optical biosensors.

HL 2.13 Mon 12:45 EW 201

**Strained Monolayer MoTe2 as a Photon Absorber in the Telecom Range** — •Muhammad Sufyan Ramzan[1] and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany. — [2]Center for Nanoscale Dynamics (CeNaD), Carl von Ossietzky Universität, 26129 Oldenburg, Germany.

For the technological application of two-dimensional (2D) materials, it is of paramount importance to understand the interplay between their electronic and structural characteristics. Using density-functional theory, we study the impact of uniaxial strain on the electronic and optical properties of monolayer $MoTe_2$[1]. Straining up to ±10% along the armchair and zigzag direction of 2D sheet, we examine how the fundamental gap, the dispersion of the bands, the frontier states, and the charge distribution are affected. Under tensile strain, the system remains a semiconductor but a direct-to-indirect band gap transition occurs above 7%. Compressive strain, instead, is highly direction-selective. When it is applied along the armchair edge, the material remains a semiconductor, while along the zigzag direction a semiconductor-to-metal transition happens above |8|%. The characteristics of the fundamental gap and wave function distribution are also largely dependent on the strain direction, as demonstrated by a thorough analysis of the band structure and of the charge density. Additional calculations based on many-body perturbation theory confirm the ability of strained $MoTe_2$ to absorb radiation in the telecom range, thus suggesting the application of this material as a photon absorber upon suitable strain modulation. [1]10.3390/nano13202740

## HL 3: Quantum Dots and Wires: Transport

Time: Monday 9:30–12:45 Location: EW 202

**Invited Talk** HL 3.1 Mon 9:30 EW 202

**Unraveling spin dynamics from charge fluctuations** — Eric Kleinherbers[1,2] and •Jürgen König[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Department of Physics and Astronomy, University of California, Los Angeles, USA

The use of single electron spins in quantum dots as qubits requires detailed knowledge about the processes involved in their initialization and operation as well as their relaxation and decoherence. In optical schemes for such spin qubits, spin-flip Raman as well as Auger processes play an important role, in addition to environment-induced spin relaxation. In [1], we demonstrate how to quantitatively extract all these rates in one go from analyzing charge fluctuations of the quantum dot measured with resonance fluorescence [2]. For this, we employ the tools of waiting-time distributions and full counting statistics characterized by factorial cumulants and discuss the role of detector imperfections [3].

[1] E. Kleinherbers et al., Phys. Rev. Res. **5**, 043102 (2023).
[2] A. Kurzmann et al., Phys. Rev. Lett. **122**, 247403 (2019).
[3] E. Kleinherbers et al., Phys. Rev. Lett. **128**, 087701 (2022).

HL 3.2 Mon 10:00 EW 202

**Coupling a single spin to high-frequency motion** — Federico Fedele[1], •Federico Cerisola[1,2], L. Bresque[3], F. Vigneau[1], J. Monsel[4], A. Palyi[5], J. Anders[2,6], and Natalia Ares[1] — [1]Univ. of Oxford, Oxford, UK — [2]Univ. of Exeter, Exeter, UK — [3]Univ. Grenoble Alpes, CNRS, Grenoble, France — [4]Chalmers Univ. of Technology, Göteborg, Sweden — [5]Budapest Univ. of Technology, Budapest, Hungary — [6]Univ. of Potsdam, Potsdam, Germany

Coupling a single spin to mechanical motion is exciting from a fundamental perspective and is also at the heart of applications such as quantum sensing, long-distance spin-spin coupling, and classical and quantum information processing. Previous experiments have observed such coupling in low-frequency mechanical resonators that are mostly confined to the classical regime, such as diamond cantilevers. Here we report the first experimental demonstration of spin-mechanical coupling with a high-frequency resonator. We achieve this all-electrically on a fully suspended carbon nanotube device. A new mechanism gives rise to this coupling, which stems from spin-orbit coupling, and it is not mediated by strain. We observe both resonant and off-resonant coupling as a shift and broadening of the electron dipole spin resonance, respectively. We develop a complete theoretical model taking into account the tensor form of the coupling and non-linearity in the motion. Our results advance spin-mechanical platforms to an uncharted regime, with promising applications ranging from the operation of fully quantum engines to the demonstration of macroscopic superpositions, to quantum simulators.

HL 3.3 Mon 10:15 EW 202

**Spin-flip rates of single electrons in coupled quantum dots** — •Olfa Dani[1], Robert Hussein[2], Johannes C. Bayer[1], Klaus Pierz[3], Sigmund Kohler[4], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hanover, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

Spin-flips are one of the limiting factors for spin-based information processing. We study electron transport through asymmetrically coupled InAs double quantum dots, demonstrating an approach for determining the spin-flip rates in such devices. Due to the different Landé-factors of the two quantum dots, the Zeeman splitting becomes inhomogeneous so that two spin channels are never resonant simultaneously. This leads to a spin-dependent blockade mechanism for single electrons at low temperatures. An electron may be trapped in the off-resonant channel and block transport until a spin flip occurs. We analyzed this blockade in terms of spin flips for different temperatures and magnetic fields and we were able to directly extract the spin-flip rates for single spins in coupled quantum dots from the measured resonant tunnel currents [1].

[1] Dani, O., Hussein, R., Bayer, J. C., Pierz, K., Kohler, S., Haug, R. J., Direct measurement of spin-flip rates in single-electron tunneling, arXiv:2310.11259 (2023)

HL 3.4 Mon 10:30 EW 202

**Impact of competing energy scales on the shell-filling sequence in elliptic bilayer graphene quantum dots** — •Lucca Valerius[1], Samuel Möller[1,2], Luca Banszerus[1,2], Angelika Knothe[3], Katrin Hecker[1,2], Eike Icking[1,2], Kenji Watanabe[4], Takashi Taniguchi[5], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen, Germany — [2]Peter Grünberg Institute, FZ Jülich, Germany — [3]Institut für Theoretische Physik, Universität Regensburg, Germany — [4]Research Center for Functional Materials, NIMS,

Tsukuba, Japan — [5]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

We investigate the shell-filling sequence of gate-defined elliptic bilayer graphene quantum dots (QDs) with low charge carrier occupation ($N \leq 12$), using magnetotransport spectroscopy and numerical calculations. Considering short-range electron-electron interactions and wave-function-dependent valley g-factors, we deepen our understanding of the fourfold shell-filling sequence, emphasizing the need to include these factors. They introduce an additional energy splitting at half filling of each orbital state, and different energy shifts in out-of-plane magnetic fields. Our analysis of 31 bilayer graphene QDs shows that the valley g-factor and energy splitting increase as QD size decreases, aligning with theoretical predictions. The charging energy of these QDs does not consistently correlate with size, revealing complex electrostatics and offering insights for future BLG QD devices.

HL 3.5 Mon 10:45 EW 202

**Electron dynamics of the inter Coulombic decay in higher excited states** — •Sara Marando[1,3] and Annika Bande[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 10409 Berlin, Germany — [2]Institute of Inorganic Chemistry, Leibniz University Hannover, Callinstr. 9, 30167 Hannover, Germany — [3]Institute of Chemistry and Biochemistry, Freie Universität Berlin, Arnimallee 22, 14195 Berlin, Germany

Quantum dots (QDs) are semiconducting nanoparticles important due to their size-tunable excitation energy and optical properties: in their self-assembled form they can host electronic or spin qubit states with a decent lifetime . To model electronic processes like the interatomic Coulombic decay (ICD) , in QDs, we apply the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm in an antisymmetrized version. ICD is described as a decay process between two or more atomic species facilitated by the long-range Coulomb interaction between electrons at different spatial locations: on the one hand, an electron in a high energy state relaxes to a lower energy state while the energy is transferred to an electron neighbour, which is simultaneously ionised. The system studied in this work consists of a one-dimensional double-well GaAs potential. It is modeled to accommodate different electronic levels (s to d energy levels) and allows ICD to occur among higher excited states.

**15 min. break**

HL 3.6 Mon 11:15 EW 202

**Study of non-linear dynamics of a nanomechanical resonator with single-electron tunneling** — •Sofia Sevitz[1], Kushagra Aggarwal[2], Janet Anders[1,3], and Natalia Ares[4] — [1]University of Potsdam, Institute of Physics and Astronomy, 14476 Potsdam, Germany — [2]Department of Materials, University of Oxford, Oxford OX1 3PH, United Kingdom — [3]Physics and Astronomy, University of Exeter, Exeter EX4 4QL, United Kingdom — [4]Department of Engineering Science, University of Oxford, Oxford OX1 3PJ, United Kingdom

Devices that present non-linear behaviour are of much interest for their broad applications ranging from thermodynamics, chaos to metrology. A promising platform is a suspended Carbon Nanotube (CNT) containing an electrostatically defined quantum dot. The electronic transport couples to the mechanical degrees of freedom of the CNT. When the coupling is in the ultrastrong regime, the CNT experiences a pronounced back-action that leads to non-linear dynamics. When the CNT is driven weakly, this non-linearity is presented as a softening of the resonance frequency of the CNT. However, when the CNT is subjected to a strong driving, intrinsic non-linearities of the mechanics take over. The main feature is the emergence of arch-like resonances in the electronic transport. In this talk, we describe our physical model that captures the combined interplay between the intrinsic non-linearities of the mechanics (modeled as a Duffing oscillator) and the electromechanical coupling under different driving regimes. Finally, we show that our model is in good agreement with our experimental electron transport measurements.

HL 3.7 Mon 11:30 EW 202

**Size distribution determines the charge transport in ZnO quantum dot (QD) materials** — •Morteza Shokrani, Dorothea Scheunemann, Clemens Göhler, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials Heidelberg University, 69120 Heidelberg, Germany

QD solids, often referred to as artificial atoms, offer the potential to create new materials with tunable macroscopic properties. Indeed, the investigation of the electronic properties of such QD assemblies has attracted attention due to the increasing applications of QD arrays in both electronics and optoelectronics. In literature, charge transport in QD assemblies has been explained by a variety of mutually exclusive theories, with the Mott and Efros-Shklovskii variable range hopping models being the most common. However, these theories fall short in explaining the anomalous exponents of the temperature-dependent conductivity $\propto \exp\left(-\left(\frac{T_0}{T}\right)^{\gamma}\right)$ observed in various QD materials. Here, we measure the temperature dependent conductivity of ZnO QDs under different UV illumination intensity. Regulating the UV intensity allows us to systematically change the effective diameter of the ZnO QDs without having to rely on cumbersome size control by synthesis. Instead, the UV level controls the width of the QD depletion shell and therefore the size distribution in the overall material. We observe exponents that systematically increase from $\gamma = 0.25$ to $\gamma = 0.75$ with increasing illumination intensity, which we interpret in terms of a charge transport being limited by the (size-dependent) charging energy of the QDs.

HL 3.8 Mon 11:45 EW 202

**Coherent Charge Oscillations in a Bilayer Graphene Double Quantum Dot** — •Katrin Hecker[1,2], Luca Banszerus[1,2], Aaron Schäpers[1], Samuel Möller[1,2], Anton Peters[1], Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Christian Volk[1,2], and Christian Stampfer[1,2] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Research Center For Functional Materials, NIMS Tsukuba, Japan — [4]International Center for Matertial Nanoarchitronics, NIMS Tsukuba, Japan

The coherent dynamics of a quantum mechanical two-level system passing through an anti-crossing of two energy levels can give rise to Landau-Zener-Stückelberg-Majorana (LZSM) interference. LZSM interference spectroscopy has proven to be a fruitful tool to investigate charge noise and charge decoherence in semiconductor quantum dots (QDs). Recently, bilayer graphene has emerged as a promising platform for highly tunable QDs potentially useful for hosting spin and valley qubits. So far, coherent oscillations have not been observed in this system and little is known about charge noise in this material. Here, we report coherent charge oscillations and T2* charge decoherence times in a bilayer graphene double QD. The charge decoherence times are independently measured using LZSM interference and photon assisted tunneling. Both techniques yield T2* average values ranging from 400 to 500 ps. The observation of charge coherence allows to study the origin and spectral distribution of charge noise in future experiments.

HL 3.9 Mon 12:00 EW 202

**Dynamics of hot carriers in core-shell InGaAs/InAlAs nanowires** — •Nabi Isaev[1], Hamidreza Esmaielpour[1], Jayesh Solomon Dayal[1], Imam Makhfudz[2], Markus Döblinger[3], Jonathan J. Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany. — [2]IM2NP, UMR CNRS 7334, Aix-Marseille Université, Marseille 13013, France. — [3]Department of Chemistry, Ludwig-Maximilians-University Munich, Munich, 81377, Germany.

The study of hot carrier dynamics in nanowires is of significant importance for advanced concept photovoltaic solar cells, such as hot carrier solar cells, which aim to improve the efficiency of this technology beyond the upper theoretical limit for single junction devices. The one-dimensional geometry of nanowires can improve the effects of hot carriers by confining them spatially, and increase photo-absorption by increasing internal reflection. Here we present our results on hot carrier dynamics in core-shell InGaAs/InAlAs nanowires grown by molecular beam epitaxy using a catalyst-free growth method. Microphotoluminescence spectroscopy has shown evidence of hot carrier effects in these nanowires. Furthermore, strong structural and dimensional dependencies in hot carrier properties were observed for these nanowires with diameters ranging from 110 nm to 200 nm. The origin of this effect is attributed to the influence of phonon bottleneck effects, Auger recombination and structural properties of the nanowires on hot carriers.

HL 3.10 Mon 12:15 EW 202

**Silicon Nanowire Transistors: Device Characteristics to Sensing Applications** — •Sayantan Ghosh[1,2], Ahmad Echresh[1], Ul-

rich Kentsch[1], Slawomir Prucnal[1], Vaishali Vardhan[3], Subhajit Biswas[3], Justin Holmes[3], 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]TU Dresden, Dresden, Germany — [3]School of Chemistry, University College Cork, Cork, Ireland — [4]Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Field-effect transistors based on silicon nanowires have been extensively used for sensing applications since the compact nanoscale structures allow excellent regulation of electrostatic potential across the nanowire channel. Sensors based on Junctionless Nanowire Transistors (JNT) have shown excellent sensitivity in liquid phases but they have not yet been operated in the gas phase.

In this work, we report the fabrication and characterisation of silicon-based JNT devices and their initial tests as gas sensors. Silicon-on-insulator wafers are doped by ion implantation and flash lamp annealing. Device patterning is based on electron beam lithography, inductively-coupled reactive ion etching, metal deposition and lift-off.

JNT sensor tests exhibited characteristic shifts in the transfer curve and a systematic increase and decrease of p- and n-type current, respectively, under the influence of different gases like NO2 and NH3 confirming potential suitability as gas sensors for detecting atmospheric radicals.

HL 3.11 Mon 12:30 EW 202

**frequency effect on channel blockade in a two- path gate-defined quantum dot** — •hatef ghannadi maragheh[1], johannes c. bayer[1], nikolai spitzer[2], arne ludwig[2], and rolf j. haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hanover, Germany — [2]Ruhr-Universität Bochum, Lehrstuhl für angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum, Germany

Knowing how any quantum device, like semiconductor-based qubit, is functioning under any condition is of vital importance to characterizing nano devices. This would be more difficult in case the structure of the device gets complicated. The device under the investigation consists of split-gate quantum dots in a GaAs/AlGaAs heterostructure where one side has a quantum dot while the other side is free. The frequency of the measurement ranged from 280 Hz to 1980 Hz.

Electron transport through the quantum dot system has been investigated for different conditions [1] including frequency [2,3] and two path cases [4,5]. For two path case, while one side has higher probability for electron transport compare to the other side, as the frequency changes, the transport behavior of the free side also changes due to the fact that the conductivity of the quantum dot is influenced by the frequency. But, these changes become less explicit as the number of electrons in the quantum dot is reduced. Furthermore, the correspondence between differential conductance for a fixed value for the plunger gate for both sides, has been investigated.

## HL 4: Perovskite and Photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00 Location: EW 203

HL 4.1 Mon 9:30 EW 203

**Improving Performance of Two-Step Processed Perovskite Top Cells for Tandem Photovoltaic Applications** — •Ronja Pappenberger[1,2], Alexander Diercks[2], Julian Petry[1,2], Paul Fassl[1,2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany

For high-performance application of perovskite solar cells (PSCs) in monolithic perovskite/silicon tandem configuration, an optimal bandgap and process method of the perovskite top cell is required. While the two-step method leads to regular perovskite film crystallization, engineering wider bandgaps ($E_g > 1.65$ eV) for the solution-based two-step method remains a challenge. This work introduces an effective and facile strategy to increase the bandgap of two-step solution-processed perovskite films by incorporating bromide in both deposition steps, the inorganic (step 1, $PbBr_2$) and the organic (step 2, FABr) precursor deposition. This strategy yields improved charge carrier extraction and quasi-Fermi level splitting with PCEs up to 15.9%. Further improvements are achieved by introducing CsI in the bulk and utilizing LiF as surface passivation, resulting in a stable power output exceeding 18.9% for $E_g = 1.68$ eV. This additional performance boost arises from enhanced perovskite film crystallization, leading to improved charge carrier extraction. Laboratory scale planar monolithic perovskite/silicon tandem solar cells (TSCs) (1 $cm^2$ active area) achieve PCEs up to 25.7%. In addition, research is being conducted into implementation on textured monolithic perovskite/silicon TSCs.

HL 4.2 Mon 9:45 EW 203

**Optical In-Situ spectroscopy and reactive spin coating for improved control of perovskite thin film fabrication** — •Simon Biberger, Maximilian Spies, Konstantin Schötz, Frank-Julian Kahle, Nico Leupold, Ralf Moos, Helen Grüninger, Anna Köhler, and Fabian Panzer — University of Bayreuth, Bayreuth, Germany

Efficient solar cells require a high-quality halide perovskite (HP) film, which is typically achieved through a solution-based solvent engineering spin coating approach. Here, HP crystallization is induced by applying an antisolvent (AS) to the precursor solution film on the spinning substrate after a specific spinning time. The process involves various controllable and uncontrollable parameters that need to be considered. As a result, fabrication recipes (such as spin speed or timing of AS dispensing) are usually developed empirically and vary between labs. Additionally, factors like changes in the atmosphere that are hard to control can introduce substantial variations between and even within batches of devices. In this work we developed a closed-loop feedback system based on our multimodal optical In-Situ spin coater system in combination with a real-time analysis of the optical spectra during spin coating. We monitor the solvent layer thickness as the parameter of interest during the spin coating. When the target level is reached, the HP crystallization is induced by dispensing the AS via a syringe pump. This method compensates for the effects of uncontrolled parameters, like variation in solvent evaporation rate due to atmospheric changes, thus leading to reproducible film quality.

HL 4.3 Mon 10:00 EW 203

**Enhanced Circular Dichroism and Polarized Emission in an Achiral, Low Bandgap Bismuth Iodide Perovskite** — •Philip Klement[1], Jakob Möbs[2], Gina Stuhrmann[3], Lukas Gümbel[1], Marius Müller[1], Johanna Heine[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Department of Chemistry, PUM, Marburg, Germany — [3]Institute of Nanotechnology (INT), KIT, Eggenstein-Leopoldshafen, Germany

Lead halide perovskites and related materials incorporating chiral organic cations exhibit intriguing properties such as chiroptical activity and chirality-induced spin selectivity enabling the generation and detection of circularly polarized light. However, understanding the structural origin of chiroptical activity presents a challenge due to macroscopic factors and experimental constraints. Here, we present the achiral perovskite derivative $[Cu_2(pyz)_3(MeCN)_2][Bi_3I_{11}]$ (pyz = pyrazine; MeCN = acetonitrile), which displays remarkable circular dichroism (CD) arising from the material*s noncentrosymmetric structure. CuBiI exhibits a low, direct optical band gap of 1.70 eV and both linear and circular optical activity with a substantial anisotropy factor of up to 0.16. Intriguingly, despite the absence of chiral building blocks, CuBiI exhibits a substantial degree of circularly polarized photoluminescence, reaching 4.9%. This value is comparable to the results achieved by incorporating chiral organic molecules into perovskites, typically ranging from 3 to 10% at zero magnetic field. Our findings shed light on the macroscopic origin of CD and provide valuable insights for the design of materials with high chiroptical activity.

HL 4.4 Mon 10:15 EW 203

**Explaining the tetragonal distortion of chalcopyrites and solving the puzzle of the peculiar bond length dependence in (Ag,Cu)(In,Ga)$Se_2$** — •Hans H. Falk[1], Stefanie Eckner[1], Konrad Ritter[1], Sergiu Levcenko[1], Timo Pfeiffelmann[1], Edmund Welter[2], Jes Larsen[3], William N. Shafarman[4], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron

DESY, Hamburg, Germany — [3]Department of Materials Science and Engineering, Uppsala University, Sweden — [4]Department of Materials Science and Engineering, University of Delaware, Newark, USA

(Ag,Cu)(In,Ga)$Se_2$ is a highly efficient thin film solar cell absorber. EXAFS studies of (Ag,Cu)$InSe_2$ and (Ag,Cu)$GaSe_2$ show that the element specific bond length of the common cation (In-Se or Ga-Se) decreases with increasing Ag content even though the lattice expands. This peculiar bond length dependence is not only counter-intuitive but also the opposite of what is commonly observed in other chalcopyrite alloys, like Cu(In,Ga)$Se_2$ and Ag(In,Ga)$Se_2$, where the bond length of the common cation (Cu-Se or Ag-Se) increases as the lattice expands. This puzzling difference in the behavior of the common cation bond lengths can be explained by minimizing the distortion energy (Keating potential) of bond angles and bond lengths. With simple calculations, focusing on the local tetrahedral neighborhood, we are able to reproduce both the tetragonal distortion and the bond length behavior of various chalcopyrite alloys, leading to a deepened understanding of these technologically relevant photovoltaic absorber materials.

HL 4.5 Mon 10:30 EW 203

**Nonlocal many-body dispersion for bulk properties: The particular case of cesium-based halide perovskites** — Lin Yang[1], Ya Gao[1], Jingrui Li[2], •Guo-Xu Zhang[1], and Zhenbo Wang[1] — [1]Harbin Institute of Technology, Harbin, P. R. China — [2]Xi'an Jiaotong University, Xi'an, P. R. China

Cesium-based all-inorganic halide perovskites have shown excellent photovoltaic properties. However, phase stability and transformations in different polymorphs remain rather poorly understood. Here, we investigate the cohesive, electronic properties and structural instabilities of $CsPbI_3$ and $CsSnI_3$ based on first-principles density-functional theory (DFT) calculations. Care has been taken to choose exchange-correlation functionals and zero-point vibrational effects have been included by performing phonon calculations. In particular, we compare different van der Waals (vdW) corrections to the DFT approaches. Our results demonstrate that nonlocal many-body dispersion interactions play a vital role in predicting the cohesive properties and phonon spectra of halide perovskites studies here. In addition, we find the anharmonicity cannot be neglected in order to correctly predict the phase stability and transitions of polymorphs. The quasiharmonic approximation method that partially include the anharmonicity is able to improve the predictions, in particular for $CsSnI_3$. We stress that both nonlocal many-body dispersion and full anharmonic terms should be considered for accurate studies of such type of materials.

HL 4.6 Mon 10:45 EW 203

**Changes in Polarization Mechanisms Following Dimensional Reduction of the Double Perovskite Octahedral Network in $Cs_2AgBiBr_6$** — •Tim P. Schneider, Jonas Glaser, Jonas Horn, and Derck Schlettwein — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen

Introduction of large organic cations into metal halide perovskites leads to dimensional reduction of the octahedral metal-halide network towards so-called 2D-perovskites with significant changes in the electronic system. Such 2D-perovskites are recently studied to enhance the performance of perovskite solar cells by reducing hysteretic behavior and improving the contact formation of perovskite absorbing layers to transport layers. In this work, 2D $PEA_4AgBiBr_8$ is derived from its 3D counterpart $Cs_2AgBiBr_6$ by replacing $Cs^+$ by the large organic phenethylammonium ($PEA^+$) cation. Thin films of both materials, 3D $Cs_2AgBiBr_6$ or 2D $PEA_4AgBiBr_8$, were prepared onto microstructured metal electrode arrays to perform *I-U* measurements and spatially resolved Kelvin probe force microscopy. These experiments serve to characterize the contact formation of both materials and discuss hysteresis caused by ion migration in response to an applied electric field. It was revealed how the dimensional reduction of the octahedral network affects the polarization caused by ionic movements and the formation of contact resistances in the films and at the respective interface to the metal electrodes. Differences among the materials, implications for technical applications in devices and the respective origin of the different observed polarization phenomena will be discussed.

**15 min. break**

**Invited Talk** HL 4.7 Mon 11:15 EW 203

**Influence of the Organic Cation Orientation on the Absorption Spectra of 2D Hybrid Organic-Inorganic Perovskites** — •Svenja Janke — Department of Chemistry, University of Warwick, Coventry, UK

Hybrid organic-inorganic perovskites (HOIPs) allow combining organic and inorganic materials at the nanoscale and hence open up a wide area of tunability. In two-dimensional HOIPs, both organic and inorganic components can contribute to the electronic frontier levels. For the design of new devices like solar cells, a fundamental understanding of the electronic excitations, their photophysical signatures and the underlying atomic structure is essential. The 2D HOIP inorganic exciton binding energy depends approximately linearly on the inorganic band gap. To estimate the inorganic exciton contribution to the absorption spectrum, I benchmark the amount of Hartree Fock exchange in hybrid density functional theory calculations including spin-orbit coupling.

For the quaterthiophene-based 2D HOIP (AE4T)$PbX_4$, variation of the halide anion leads to structural changes in the organic layer, causing changes in the absorption spectra. The bithiophene-based 2D HOIP (AE2T)$PbI_4$ shows disorder along the stacking direction in X-ray scattering experiments, resulting in several possible atomic structural models for the organic component.

Here, I demonstrate that we can use a Frenkel-Holstein-Hamiltonian-based model to investigate how different orientations of the organic cation alter the organic and inorganic exciton contribution to the absorption spectrum.

HL 4.8 Mon 11:45 EW 203

**Optical Simulations of Light Management in Ultrathin CIGSe Solar Cells with Nanophotonic Back Contacts** — •Daniel Jimenez Tejero, Merve Demir, Thomas Schneider, Bodo Fuhrmann, Roland Scheer, Ralf Wehrspohn, and Alexander Sprafke — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale), Germany

Ultrathin Cu(In,Ga)$Se_2$ (CIGSe) solar cells are in development to decrease material usage and broaden the range of applications. However, CIGSe absorber layers with thicknesses below 1 $\mu$m suffer from reduced light absorption, especially for wavelengths near the bandgap, leading to decreased power conversion efficiency. To counteract this, we employ nanostructured functional back contacts to effectively increase the optical path length within the CIGSe absorber layer through nanophotonic mechanisms such as scattering and coupling into thin film modes. The focus lies on CIGSe absorber layers with a thickness of 300 nm to 500 nm deposited on $SiO_2$ nanostructures on a flat aluminium or gold back contact. Our approach employs nano-optical simulations using the finite element method and aims to identify designs with promising photocurrent enhancements feasible for fabrication and to clarify the underlying mechanisms.

HL 4.9 Mon 12:00 EW 203

**Multi-Phase Optical Exciton Dynamics in Mixed (2D/3D) Inorganic-Organic Hybrid Semiconductors** — •Mohammad Adnan[1,2], Pawan Kumar Kanaujia[2], Kshetra Mohan Dehury[2], and Gaddam Vijaya Prakash[2] — [1]Institute of Physics, University of Münster, Wilhelm-Klemm-Straße 10 48149 Münster, Germany — [2]Nanophotonics Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India

Inorganic-organic (IO) hybrid semiconductors are promising optoelectronic materials due to their unique crystal packing, the wide variety of crystal phases, the wide bandgap tunability and the associated optical exciton characteristics. Here, we investigate the digitized intercalation process of various organic moieties, resulting in a mixed IO hybrid system of type (R-NH3)2(R'-NH3)n-1PbnI3n+1. By employing continuous photoluminescence monitoring, we observe a progressive and dynamic structural evolution and elucidate the underlying mechanisms occurring during the intercalation process. The interplay of (i) cyclic (ii) long alkyl chain and (iii) small alkyl amine based organic moieties during the intercalation leads to the formation of either 2D ((R-NH3)2PbI4) or 3D (R'-NH3PbI3) IO hybrid networks and causes significant structural phase variations within the 2D and 3D crystal packings.

HL 4.10 Mon 12:15 EW 203

**Exploring Mixed-Metal Chalcohalides $M(II)_2M(III)Ch_2X_3$ Compounds for Photovoltaic Applications** — •Pascal Henkel[1], Jingrui Li[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, P.O.Box 11100, FI-00076 AALTO, Finland — [2]School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China

New photovoltaic materials are needed to increase power conversion efficiencies (PCEs), reduce costs, and improve device longevity to facilitate the renewable energy transformation. In this context, perovskite-inspired quaternary mixed-metal chalcohalides $M(II)_2M(III)Ch_2X_3$ have emerged as an interesting materials class, that has the potential to overcome the stability and toxicity problems of the currently favoured halid perovskites [1], and still deliver high PCEs [2].

In this study, we apply density functional theory to identify new $M(II)_2M(III)Ch_2X_3$ compounds. We considered a total of 54 materials each in three different space groups ($Cmcm$, $Cmc2_1$ and $P2_1/c$) for which we computed the energetic stability and the band gaps with the HSE06 hybrid functional. We identified a total of 22 $M(II)_2M(III)Ch_2X_3$ materials, which fulfill our stability requirements and have a direct band gap in the range 0.7 eV to 2 eV. Out of the 22, 8 lead-free and 9 lead-containing materials are new [3]. Overall for all 54 compounds, $P2_1/c$ is the thermodynamically preferred phase, whereas direct band gaps occur predominantly for $Cmcm$ and $Cmc2_1$.

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

HL 4.11 Mon 12:30 EW 203

**Effective model for charge transport in hybrid organic-inorganic materials dominated by molecule-lattice interactions** — •Florian Kluibenschedl, Georgios Koutentakis, Ragheed Alhyder, and Mikhail Lemeshko — Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria

The growing importance of crystalline hybrid materials with embedded molecular entities, such as hybrid organic-inorganic perovskites (HOIPs) or molecular organic frameworks, requires extensions of the conventional picture of charge transport based on electron-phonon interactions. Here we present a minimal, coarse-grained, two-dimensional model of charge transport based on the interactions of charge carriers with freely rotating molecules embedded in the inorganic lattice. Our phase diagram analysis reveals the presence of four phases, characterized by the distinct ordering of the molecular dipole moments, which strongly depends on the tunneling anisotropy of the carriers as well as on the strength of carrier-molecule interactions. The most striking outcome is the coexistence of degenerate ferroelectric phases of reduced symmetry beyond a certain threshold of interaction strength, even in the case of isotropic tunneling. The coexistence of these phases motivates a symmetry breaking mechanism similar to the Jahn-Teller effect, which introduces transport anisotropy into an otherwise symmetric system. We relate these results to the proposed formation of ferroelectric large polarons as an explanation of the remarkable optoelectronic properties of HOIPs.

HL 4.12 Mon 12:45 EW 203

**Cavity-enhanced absorption measurements of perovskite nanocrystals** — •Ines Amersdorffer[1], Andreas Singldinger[1], Thomas Hümmer[1,2], Alexander Urban[1], and David Hunger[3] — [1]Faculty of physics, LMU Munich, Germany — [2]Qlibri GmbH, Munich, Germany — [3]Physikalisches Institut, KIT, Germany

The search for optimal materials for optoelectronic devices such as solar cells or quantum light emitters has piqued significant interest in perovskite nanocrystals. This is due to their outstanding properties, which range from easy, scalable synthesis at room temperature to ultra-wide colour tunability and high quantum efficiency.

Spectroscopy on single perovskite crystals helps to reveal their excitonic fine structure, which in thin films is concealed by inter-particle phenomena. However, measuring the marginal absorption of such nanocrystals is challenging. One way to overcome this issue is to use an optical resonator in which the light passes through the nanoscale sample multiple times and thereby enhances its absorption to a measurable amount.

To this end, we use a high-finesse microcavity to perform wavelength dependent absorption measurements on perovskite nanocubes. These are complemented by low-temperature photoluminescence and scanning electron microscopy images. The combination of these techniques will provide unprecedented insight into the size- and morphology dependence of the energetic structure of individual nanocrystals. The results show progress towards routine hyperspectral absorption measurements at the nanoscale.

## HL 5: Optical Properties I

Time: Monday 9:30–11:45 Location: EW 561

HL 5.1 Mon 9:30 EW 561

**Can we predict exciton binding energies from ground-state properties?** — •Malte Grunert, Max Grossmann, and Erich Runge — Theoretische Physik I, TU Ilmenau, Germany

Accurate ab-initio exciton binding energies are commonly obtained by solving the Bethe-Salpeter equation on the results of an expensive quasiparticle calculation. Accurate ground-state properties, however, are often much cheaper to evaluate. Establishing reliable connections between cheap ground-state properties and expensive exciton binding energies is therefore desirable - ideally, we would be able to predict the latter based on the former!

A well-known method of predicting exciton binding energies is the Wannier-Mott model, which is however not directly applicable to more localized excitons. Several alternative approaches have been put forward proposing that e.g., the colocalization of electron and hole states [1] or a high JDOS around the bandgap [2] correlates with increasing exciton binding strength.

We investigate and possibly verify these proposed links between exciton binding energies and ground-state properties in several dozen materials across different classes of materials, including simple narrow- and wide-bandgap semiconductors, insulators, and more complex compounds such as transition metal chalcogenides and perovskites. We critically evaluate emerging trends and attempt predictions going beyond the Wannier-Mott model.

[1] M. Dvorak et al., Phys. Rev. Lett., 2013, 110, 016402
[2] E. Baldini et al., Nat. Commun. 2017, 8, 13

HL 5.2 Mon 9:45 EW 561

**Conduction band nonparabolicity, chemical potential, and carrier concentration of intrinsic InSb as a function of temperature** — •Stefan Zollner, Carlos Armenta, and Sonam Yadav — New Mexico State University, Las Cruces, NM, USA

The goal of our work is to predict the complex dielectric function of intrinsic indium antimonide from 80 to 800 K, which was recently measured using spectroscopic ellipsometry [M. Rivero Arias *et al.*, J. Vac. Sci. Technol. B **41**, 022203 (2023)]. The first step is to find a good analytical description for the nonparabolic band structure of InSb based on $\vec{k} \cdot \vec{p}$ theory. We implement a simple $8\times8$ $\vec{k} \cdot \vec{p}$ Hamiltonian based on the work of Kane (1956) within the limit of large spin-orbit splittings, where a single nonparabolicity parameter provides a good description of the density of states. We select a value of the momentum matrix element $P$ which yields the experimental effective electron mass for the unrenormalized low-temperature band gap. The temperature-dependence of the effective electron mass is then calculated taking into account only the thermal expansion contribution to the redshift of the direct band gap, not the renormalization due to deformation-potential electron phonon interactions. With this approach, we calculate the temperature dependence of the chemical potential, the thermal Burstein-Moss shift, and the carrier concentration of intrinsic InSb, which is in good agreement with electrical Hall effect measurements. The calculation of the temperature-dependent dielectric function will be the next step.

HL 5.3 Mon 10:00 EW 561

**Interplay between excitons and lattice vibrations in the optical properties of monolayer boron nitride** — •Giovanni Marini, Matteo Calandra, and Pierluigi Cudazzo — University of Trento, Department of Physics, Via Sommarive 14 Povo(TN)

Monolayer hexagonal boron nitride exhibits a complex optical response, the full understanding of which remains elusive. The photoluminescence spectrum is enriched with satellite features that hint at the existence of substantial couplings between excitons and phonons whose nature is completely unknown. Being photoluminescence experiments always performed in presence of a substrate, the knowledge of the basic properties of the isolated ideal layer constitutes fundamental

reference for the interpretation of the experiments and allows disentangling the effect of the substrate. Here, through a cumulant expansion of the charge response function developed in the framework of many body perturbation theory, we performed a first principles study of the exciton-phonon coupling in monolayer boron nitride. Our results allows to identify the different exciton-phonon scattering channels and their effect on the optical properties of this system providing important insights about recent photoluminescence experiments.

HL 5.4 Mon 10:15 EW 561

**Optical and Structural Properties of Zinc Oxide Nanoparticles using the Leaf Extract of Silybum marianum (Milk Thistle)** — •Ahed AL-Faouri[1], Mahmoud Abu-Kharma[2], and Mahmoud Hatem[3] — [1]Al-Ahliyya Amman University — [2]Al-Balqa Applied University — [3]Al-Balqa Applied University

This study utilized the leaf extract of Silybum marianum (Milk thistle), as an effective bio-reductant, stabilizer, and capping agent for the synthesis of zinc oxide nanoparticles (ZnO-NPs) at ambient temperature. The chosen approach was not only simple and efficient but also demonstrated low-cost, non-toxic, and environmentally friendly characteristics, aligning with green synthesis principles. ZnO -NPs were detected and characterized using a Fourier transform infrared spectroscopy (FTIR), UV-Visible (UV-Vis) spectroscopy, X-ray powder diffraction (XRD), and scanning electron microscope (SEM). UV-Vis spectroscopy showed a sharp peak at 373 nm, and the energy band gap was measured to be approximately 2.77 eV. Furthermore, the UV-Vis analysis was utilized to quantify and interpret a range of optical properties. These properties include the absorption coefficient ($\alpha$), skin depth ($\delta$), optical density (Dopt), extinction coefficient (k), optical conductivity ($\sigma$opt), and the optical dielectric constant ($\epsilon$). This thorough exploration of the optical and structural characteristics of the CuO-NPs aids in comprehending their response to light interaction, thereby opening avenues for their practical applications across various fields.

**15 min. break**

HL 5.5 Mon 10:45 EW 561

**Cr-doped $Ga_2O_3$ microcavities for thermometric applications** — •Ruben Johannes Theodorus Neelissen[1], Manuel Alonso-Orts[1], Daniel Carrasco[2], Marco Schowalter[1], Andreas Rosenauer[1], Emilio Nogales[2], Bianchi Mendez[2], and Martin Eickhoff[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.

Monoclinic gallium oxide ($\beta$-$Ga_2O_3$) is a transparent conductive oxide with an ultra-wide bandgap of 4.8 eV and high chemical and thermal resilience. This makes $\beta$-$Ga_2O_3$ very interesting for areas such as high power (opto)electronics.

Previous work [1] focused on chromium doped $\beta$-$Ga_2O_3$ microwires as optical microcavities and their use of thermometric application. Focused ion beam (FIB) fabricated distributed Bragg reflectors (DBRs) enhance the confined light in the microcavities, resulting in strong resonances. With increasing temperature, the resonant wavelength of these peaks redshifts due to changes in both the refractive index and the optical length of the cavities. The operation of these wide dynamic range thermometers with a resolution of 1 K was demonstrated [1].

However, the FIB-fabricated microcavities involve a complex fabrication process, are mechanically unstable and are not resilient to high laser powers. In this work, a new fabrication method involving atomic layer deposition (ALD) was developed.

[1] M. Alonso-Orts et al. In: *Small 18.1* (2022), p. 2105355.

HL 5.6 Mon 11:00 EW 561

**Carrier generation and diffusion in Ga(As,Sb) nanowires probed by cathodoluminescence spectroscopy** — •Mikel Gómez Ruiz[1], Vladimir Kaganer[1], Akhil Ajay[2], Hyowon Jeong[2], Gregor Koblmüller[2], Oliver Brandt[1], and Jonas Lähnemann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Germany — [2]Walter Schottky Institut, School of Natural Sciences, Technical University of Munich (TUM)

Semiconductor nanowire (NW) structures emitting at wavelengths used for optical telecommunications are attractive for the integration on silicon-on-insulator waveguides. Here, we study Ga(As,Sb) NWs with a lower bandgap (In,Ga)As insertion on a microscopic scale by cathodoluminescence (CL) spectroscopy to understand the charge carrier transfer to and the recombination in the insertion. In our CL experiments the electron beam, and thus the volume in which electron-hole pairs are generated, is scanned along the axis of the NW. After their generation and diffusion, the carriers recombine either in the Ga(As,Sb) segment or in the (In,Ga)As insertion, giving rise to spectrally distinct CL bands. The intensity profiles of both emission bands are recorded as a function of the beam position. Although the (In,Ga)As insertion is only about 20 nm long, the corresponding CL band can be observed over a length of more than 400 nm under high excitation conditions. The evolution of these profiles with temperature is studied to determine the diffusion length in the Ga(As,Sb) NW using a model that includes the temperature-dependent generation volume and the diffusion of the cathodogenerated carriers.

HL 5.7 Mon 11:15 EW 561

**Excitons in Helium Under Pressure** — •Fatema Mohamed[1], Frédéric Pailloux[2], Marie-Laure David[2], Laurent Pizzagalli[2], Lucia Reining[1], and Matteo Gatti[1] — [1]LSI, Ecole Polytechnique, CNRS, Palaiseau, France — [2]Institut Pprime, Université de Poitiers, Poitiers, France

The absorption and the electron energy loss spectra of solid helium at different pressures are calculated using a first principles approach based on the Bethe-Salpeter equation of many-body perturbation theory. The results are used to explain the effect of pressure on HCP helium that has been measured by spectroscopy experiments [1,2]. We found a well defined exciton peak, showing linear pressure dependence, both in the peak position and intensity. We calculated the excitonic dispersion of the loss function along the Γ-M direction for momentum transfers beyond the first Brillouin zone. We found strong parabolic-like dispersion of the spectra, dominated by the screened Coulomb interaction. Near Bragg reflection points we found an anomalous angular dependence of the exciton peak, due to the crystal local field effects, analogously to the plasmon in graphite [3].

References:
1- M.-L. David, et al. Appl. Phys. Lett. 98, 171903, 2011.
2- H. K. Mao, et al. Phys. Rev. Lett. 105, 186404, 2010.
3- R. Hambach, et al. Phys. Rev. Lett. 101, 266406, 2008.

HL 5.8 Mon 11:30 EW 561

**UV defect emitters in hexagonal boron nitride** — •Nils Bernhardt[1], Luca Choi[1], Benjamin M. Janzen[1], Felix Nippert[1], Angus Gale[2], Igor Aharonovich[2], Milos Toth[2], and Markus R. Wagner[3,1] — [1]Technische Universität Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]University of Technology Sydney, Sydeny, Australia — [3]Paul Drude Institute for Solid State Electronics, Berlin, Germany

Room temperature defect quantum emitters in hexagonal boron nitride have emerged as a source of considerable scientific interest. Recent studies have demonstrated the ability to engineer reliable single photon sources in thin film hBN with reproducible emission properties in all spectral ranges, suitable for applications such as quantum communications. While extensive studies of such emitters in hBN have been conducted in the visible and near-IR spectral range, this work aims to investigate the recently observed UV luminescence of hBN point defects at 4.1eV, likely caused by carbon substitutions at nitrogen sites.

A frequency-quadrupled titanium-sapphire laser at 200 nm is used for pulsed above-bandgap excitation and compared to sub-bandgap pulsed and continuous wave excitation. A direct dependence between the luminescence of the defect and its surroundings is explored to establish a link between the properties of the 2D material samples and the electron-phonon coupling. These results are corroborated by the correlation of AFM, micro-Raman, and micro-PL mapping measurements.

# HL 6: Semiconductor Qubits (joint session QI/HL)

Time: Monday 9:30–12:45 Location: HFT-FT 131

**Invited Talk** HL 6.1 Mon 9:30 HFT-FT 131

**Spin circuit-QED in the time-domain** — •Jurgen Dijkema[1], Xiao Xue[1], Patrick Harvey-Collard[1], Maximilian Rimbach-Russ[1], Sander L. de Snoo[1], Guoji Zheng[1], Amir Sammak[2], Giordano Scappucci[1], and Lieven M.K. Vandersypen[1] — [1]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands — [2]QuTech and Netherlands Organization for Applied Scientific Research, Delft University of Technology, Delft, The Netherlands

Semiconductor spin qubits hold promise for quantum computation due to their long coherence times and potential for scaling. So far, interactions between spin qubits are limited to spins a few hundreds of nanometers apart. A distributed architecture with local registers and long-range couplers will be needed to scale up to millions of qubits. Circuit quantum electrodynamics can provide a pathway to realize interactions between distant spins. Here, we report long-range spin-spin interactions using an on-chip superconducting resonator in two regimes. First with two spins detuned from the resonator frequency, allowing the demonstration of two-qubit iSWAP logic via virtual photons. Next, we tune the two spin frequencies to match the resonator frequency and demonstrate spin state-transfer using real resonator photons.

HL 6.2 Mon 10:00 HFT-FT 131

**Optimal electron trajectories improving the spin-shuttling fidelity beyond the adiabatic limit** — •Alessandro David[1], Lars R. Schreiber[2], Hendrik Bluhm[2], Tommaso Calarco[1], and Felix Motzoi[1] — [1]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, Jülich, Germany — [2]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany

Spin-qubit quantum computers are currently limited by a connectivity problem. A promising solution is the use of conveyor-mode shuttling architectures [1] where the qubit encoded in the spin of an electron is reliably transported by a moving quantum dot [2]. During this process the spin experiences decoherence from uncontrollable features of the device heterostructure such as interface roughness, valley degree of freedom and spin-orbit coupling [3]. In this work we compute the energy splitting of the valley with the help of an alloy-disorder model [4] and we focus on the dephasing interaction between spin and valley. Using quantum optimal control techniques we find electron trajectories that improve the spin-shuttling fidelity by reducing the valley excitation even at higher speeds than the adiabatic limit. The experimental adequacy of our results is inspected through statistical sampling of different devices and bandwidth limitation of the electron trajectories.

[1] Künne and Willmes et al., arXiv:2306.16348 (2023) [2] Struck et al., arXiv:2307.04897 (2023) [3] Langrock and Krzywda et al., PRX Quantum 4, 020305 (2023) [4] Wuetz, et al., Nat. Comm. 13, 7730 (2022)

HL 6.3 Mon 10:15 HFT-FT 131

**Counteracting decoherence induced by spin-valley coupling in single-qubit manipulation zones via quantum optimal control** — •Akshay Menon Pazhedath[1], Alessandro David[1], Lars R. Schreiber[2], Tommaso Calarco[1], Matthias M. Müller[1], Hendrik Bluhm[2], and Felix Motzoi[1] — [1]Peter Grünberg Institute-Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany

Quantum bus architectures based on electron spin shuttling in a Si/SiGe heterostructure are promising candidates for scalable quantum computing. Electrically controlled single qubit gates are achieved with a carefully placed micro-magnet that provides a synthetic spin-orbit coupling in the designated manipulation zones [Künne et al. arXiv:2306.16348 (2023)]. The presence of spin-valley mediated decoherence hotspots at the vicinity of the micro-magnet can cause spin decoherence, limiting the capability to achieve fault tolerant gates. Using quantum optimal control techniques, we obtain new electron trajectories leading to significant improvements to the gate fidelity. The influence of valley splitting and the distance from decoherence hotspots are also investigated, based on statistical sampling of prototypical device configurations. For increasing values of spin-valley coupling, 99.12% of the samples converged below the required fault tolerant gate fidelity threshold, where all of the under- performing samples are due to a high value of spin-valley coupling.

**Invited Talk** HL 6.4 Mon 10:30 HFT-FT 131

**Gate defined electron and hole quantum dots in bilayer graphene** — •Luca Banszerus — Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany

Bilayer graphene (BLG) quantum dots (QDs) have long been regarded as an attractive platform for hosting spin qubits since the low nuclear spin densities and weak spin-orbit interaction in BLG promise long spin coherence times. In addition to the spin, BLG exhibits a tunable valley degree of freedom, which is associated with a strong out-of-plane magnetic moment with opposite signs for the K- and K'-valley. This allows controlling the valley splitting in BLG and to use valley space as an additional qubit platform.

In contrast to conventional semiconductors, the band structure of BLG is (almost) perfectly electron/hole symmetric and exhibits an electrically tuneable band gap, which we use to form ambipolar electron/hole double QDs. We observe the creation of single electron-hole pairs with opposite quantum numbers and use the electron-hole symmetry to achieve a protected spin-valley blockade in electron-hole double quantum dots. The latter allows for spin-to-charge conversion and valley-to-charge conversion, which is essential for the operation of spin and valley qubits.

HL 6.5 Mon 11:00 HFT-FT 131

**Spin and valley relaxation in a single-electron bilayer graphene quantum dot** — •Lin Wang and Guido Burkard — Department of Physics, University of Konstanz, D-78457, Germany

Bernal-stacked bilayer graphene (BLG) has a tunable gap controlled by an out-of-plane electric field. This makes BLG a possible candidate to form quantum dots (QDs). Spin-based qubits in BLG QDs have received great attention due to the low spin-orbit interaction and low hyperfine coupling. Long spin relaxation times of a single-electron state in BLG QDs was recently reported [1,2]. In addition to spin, valley pseudospin is another degree of freedom in BLG. The two valleys experience opposite Berry curvatures and associated magnetic moments via an out-of-plane electric field. This provides a promising way towards controlling valleys and further establish valley-based electronics and qubits. The valley relaxation time between triplets and singlets was reported to be remarkably long in BLG double QDs [3]. To assess the potential of spin/valley qubits, the spin/valley relaxation time is a crucial parameter since it directly limits the lifetime of encoded information. Here, we theoretically investigate the spin/valley relaxation in a single-electron BLG QD due to spin-orbit/intervalley coupling assisted by (i) 1/f charge noise and (ii) electron-phonon couplings arising from the deformation potential and the bond-length change. Detailed comparisons with the existing experiments on both spin and valley relaxation times are shown. [1]L. Banszerus et al., Nat. Commun. 13, 3637 (2022). [2]L. M. Gächter et al., PRX Quantum 3, 020343 (2022). [3]R. Garreis et al., arXiv:2304.00980.

**15 min. break**

HL 6.6 Mon 11:30 HFT-FT 131

**Classification and magic magnetic field directions for spin-orbit-coupled double quantum dots** — •Aritra Sen[1], Gyorgy Frank[1], Baksa Kolok[1], Jeroen Danon[2], and Andras Palyi[1] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Norwegian University of Science and Technology, Trondheim, Norway

Fundamental building blocks of spin-based quantum computing have been demonstrated in semiconductor double quantum dots with significant spin-orbit coupling. Here, we show that spin-orbit-coupled double quantum dots can be categorized in six classes, according to a partitioning of the multidimensional space of their $g$ tensors. The class determines physical characteristics of the double dot, i.e., features in transport, spectroscopy, and coherence measurements, as well as qubit control, shuttling, and readout experiments. In particular, we

predict that the spin physics is highly simplified due to pseudospin conservation, whenever the external magnetic field is pointing to special directions ('magic directions'), where the number of special directions is determined by the class. We also analyze the existence and relevance of magic loops in the space of magnetic-field directions, corresponding to equal local Zeeman splittings. These results present an important step toward precise interpretation and efficient design of spin-based quantum computing experiments in materials with strong spin-orbit coupling.

HL 6.7 Mon 11:45 HFT-FT 131

**Dynamical sweetspots in driven germanium double quantum dot spin qubits** — •Yaser Hajati and Guido Burkard — Konstanz University, Konstanz, Germany

In recent years, significant strides have been made in advancing hole-spin qubits based on semiconductor quantum dots, particularly in germanium (Ge). Hole spins in Ge quantum dots can leverage the strong spin-orbit coupling compared to silicon, potentially enabling fast and reliable qubit operations. Our study focuses on exploring the use of a periodic drive field to engineer the properties of Ge quantum-dot based qubits amidst charge noise. Specifically, we investigated the Rabi frequency of a hole qubit experiencing detuning driving in a planar Ge double quantum dot, focusing on the single-hole flopping mode with spin-orbit interaction. Our findings indicate that the Rabi frequency linked to a hole within a planar double quantum dot, driven on resonance, exhibits an inverse correlation with detuning energy while demonstrating a positive correlation with driving frequency, Zeeman field strength, and spin-orbit coupling. Furthermore, through strategic modulation of the drive frequencies slightly off resonance, we effectively mitigated the impact of charge noise. This modulation significantly boosted the fidelity of quantum gates when manipulating the qubit within specific ranges of drive frequencies and detuning. Importantly, our study shows that fidelity improvements at dynamic sweet spots exceed those achievable by solely adjusting drive frequency and detuning. Discovering these spots holds potential for enhancing quantum gate reliability in Ge quantum dot-based computing.

HL 6.8 Mon 12:00 HFT-FT 131

**Floquet Quantum Processors** — •Giovanni Francesco Diotallevi and Monica Benito — Universität Augsburg, Augsburg, Germany

Quantum dot confined hole spin qubits posses a variety of properties that render them highly attractive candidates for the development of quantum computing platforms [1]. However, using these to construct functioning large quantum processors still faces major challenges. Among these, being able to simultaneously control distant qubits with minimal cross-talk between untargetted qubits remains a goal to be achieved in the field. In this direction recent studies proposed to mediate the coupling between two distant qubits by means of superconducting quantum resonators [2].

In this research we intend to explore techniques involving external periodic drives to better control the coupling of these hole spin qubits to the interaction-mediating resonators. In particular, we envision an ensemble of periodic fields used to control the individual coupling of a series of hole spin qubits to a single resonator. Using Floquet-based theory it is indeed possible to tune the spin-orbit interaction of these qubit systems [3], thus allowing us to selectively choose which qubits to couple in order to perform desired quantum gates.

References: [1] Y. Fang et Al., *Recent advances in hole-spin qubits,* Materials for Quantum Technology, vol. 3, no. 1, p. 012003, 2023. [2] J. Dijkema et Al., *Two-qubit logic between distant spins in silicon,* 2023. [3] O. V. Kibis et Al., *Floquet engineering of the luttinger hamiltonian,* Phys. Rev. B, vol. 102, p. 035301, Jul 2020.

HL 6.9 Mon 12:15 HFT-FT 131

**Quantum Gates with Oscillating Exchange Interaction** — •Daniel Nguyen, Irina Heinz, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Two-qubit gates between spin qubits are often performed using a rectangular or an adiabatic exchange interaction pulse resulting in a CZ gate. An oscillating exchange pulse not only performs a CZ gate, but also enables the iSWAP gate, which offers more flexibility to perform quantum algorithms. We provide a detailed description for two-qubit gates using resonant and off-resonant exchange pulses, give conditions for performing the respective gates, and compare their performance to the state-of-the-art static counterpart. We find that for relatively low charge noise the gates still perform reliably and compare to the conventional CZ gate.

D. Q. L. Nguyen, I. Heinz, and G. Burkard, Quantum gates with oscillating exchange interaction (2023), arXiv:2303.18015 [quant-ph].

HL 6.10 Mon 12:30 HFT-FT 131

**Gate operations on Exchange-Only spin qubits with oscillating drive** — •Tobias Heinz, Stephen R. McMillan, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

A major obstacle on the path towards large-scale quantum computing lies in achieving high fidelities for gate operations. Spin qubits using exchange interaction alone have emerged as promising candidates [1] due to their resistance to certain types of decoherence [2]. Motivated by the proposed gate of Doherty and Wardrop [3], this work focuses on the application of an oscillating drive field to facilitate an entangling two qubit operation between two local Resonant-Exchange qubits. By driving the exchange interaction belonging to one qubit, we propose a CNOT gate for universal quantum computing, with gate times in the range of a hundred nanoseconds. We analyze the impact of the drive amplitude on gate fidelity and gate time, providing insights into the optimal parameter regimes. Through numerical simulations, we determine the impacts of leakage and off-resonant processes on the fidelity. For context, we compare our results to a static gate obtained through a dc pulse of the interqubit exchange coupling. Our proposal contributes to the understanding of the implementation of spin qubits and paves the way for the development of robust and scalable quantum computers. [1] G. Burkard et al. Rev. Mod. Phys. 95, 025003 (2023). [2] J. M. Taylor et al. Phys. Rev. Lett. 111, 050502 (2013). [3] A. C. Doherty et al. Phys. Rev. Lett. 111, 050503 (2013).

# HL 7: Transport properties I

Time: Monday 15:00–17:00 Location: ER 325

HL 7.1 Mon 15:00 ER 325

**Challenges of mapping transport parameters of N-doped 4H-SiC by Raman spectroscopy** — •Hannes Hergert[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Center for Materials Research, Giessen, Germany — [2]Instituten of Experimental Physics I, Giessen, Germany — [3]Institute of Physical Chemistry, Giessen, Germany

We assess Raman spectroscopy as a tool for fast and non-invasive mapping of charge carrier density and carrier mobility in inhomogeneously doped 4H-SiC. For this purpose, we compare values of these transport parameters obtained by magneto-transport and Raman measurements of N-doped 4H-SiC. The effective charge density and mobility, which are obtained from resistivity and Hall measurements by employing the commonly used effective one-band model, deviate from the values extracted by applying the established line-shape models for describing the longitudinal optical phonon coupled (LOPC) modes in the Raman spectra. Differentiating between free and localized carriers in the framework of a three-band transport model confirms that only the free charge carriers in the conduction band of N-doped 4H-SiC contribute to the LOPC Raman signal and their density agrees well with that obtained by the line shape analysis. The agreement of the mobility values is reasonable keeping in mind that different frequencies of the applied electric fields are used in the two approaches. Moreover, the excitation of electrons into the conduction band by the laser causes differences in the temperature dependence of the carrier density compared with the electrical transport data.

HL 7.2 Mon 15:15 ER 325

**Stoichiometry fluctuations and geometrical confinement in random alloys: a case study on SiGe:C** — •Daniel Dick[1,2,3], Florian Fuchs[1,2,3], Jörg Schuster[1,2,3], and Sibylle Gemming[3,4] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

We investigate the effect of base layer scaling in silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs) and evaluate the effect of local fluctuations in atomic concentrations using electronic structure theory.

For calculating the band structure of SiGe:C alloy with varying Ge and C content we present a new parameterization of Germanium in the framework of extended Hückel theory (EHT). Combined with the use of empirical potentials for structural relaxation, it enables us to efficiently simulate a large number of permutations of the atomic structure to quantify the influence of atomic-scale fluctuations on the electronic structure and transport properties using unit cells with more than a hundred atoms.

Comparing bulk SiGe:C alloy and thin layers gives insight on how quantum confinement and local stoichiometry fluctuations affect transport properties of ultra-scaled HBTs. Results are verified by first-principles calculations using density functional theory.

HL 7.3 Mon 15:30 ER 325

**$Ti_2MnAl$ and its modifications, as possible Spin-Gapless-Semiconductor materials.** — •Jerzy Goraus, Wojciech Gumulak, and Jacek Czerniewski — Institute of Physics, Faculty of Science and Technology , University of Silesia, 41-500 Chorzów, 75 Pułku Piechoty 1A, Poland

$Ti_2MnAl$ was earlier predicted to exhibit Spin-Gapless-Semiconductor (SGS) properties. SGS materials are very interesting due to their potential applications in spintronics. Only in one variant of crystal structure, $Ti_2MnAl$ can have such properties; this variant (as we and other researchers have already shown) is not realized in nature. There were, however, papers claiming that element substitution of $Ti_2MnAl$ could stabilize inverse Heusler structure for which SGS state is possible. In that presentation, we report our results for studies of $Ti_2MnAl$ where Al was substituted by In or Sn, as well as for the isoelectronic $Ti_2Fe_{0.5}Cr_{0.5}Al$ compound. We show the results of our experimental measurements - polycrystalline samples characterized with XRD technique, with their resistivity and magnetic properties measurements as well as DFT calculations of the stability of the particular unit cell. We will also show these results in the context of our earlier research of similar materials involving sample surface measurements such as XPS and XAS measurements. The latter, as shown in our earlier report for $Ti_2CrAl$ can also resolve the unit cell structure, which is difficult for these materials by the XRD technique alone.

HL 7.4 Mon 15:45 ER 325

**Electrical Conductivity and Carrier Mobility for Strongly Anharmonic Materials from First Principles** — •Jingkai Quan[1,2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195, Berlin, Germany — [2]Max-Planck Institute for the Structure and Dynamics of Matter, Luruper Chausse 149, 22761, Hamburg, Germany

First-principle approaches for describing phonon-limited electronic transport are typically based on many-body perturbation theory and the Boltzmann transport equation, which can be questionable in strongly anharmonic systems. Combining ab initio molecular dynamics (aiMD) simulations and the Kubo-Greenwood (KG) formalism, we investigate a non-perturbative stochastic method to calculate carrier mobilities, which accounts for all orders of anharmonic and vibronic couplings. We implement the KG formula in the highly efficient all-electron code FHI-aims. In particular, we discuss in this talk the definition of carrier mobility in the KG framework and the developed numerical strategies employed to overcome the notoriously slow convergence of the phase-space and Brillouin-zone integrals in crystalline solids. Using strongly anharmonic perovsktie $SrTiO_3$ and $BaTiO_3$, we demonstrate the capabilities and predictive power of the KG approach and investigate the influence of the chosen exchange-correlation functional on the obtained conductivities and mobilities. Eventually, we analyze the observed trends and explain the effects in terms of self-energy shifts and broadenings.

**15 min. break**

HL 7.5 Mon 16:15 ER 325

**Electronic Transport Properties of Janus Ge-Based Two-Dimensional IV-V Monolayer** — •Dogukan Hazar Ozbey[1], Gozde Ozbal Sargin[2], Veli Ongun Ozcelik[2], and Engin Durgun[1] — [1]Bilkent University UNAM — [2]Sabanci University

Two-dimensional (2D) semiconductors with anisotropic properties have garnered significant attention in materials research, particularly those exhibiting strong anisotropy in carrier mobility. A captivating subset of these materials is Janus monolayers, characterized by the substitution of all atoms on one side of their binary counterpart with a different element. This structural transformation disrupts the out-of-plane mirror symmetry, offering a platform for exploring extraordinary physical properties in 2D Janus crystals. In this study, we present a comprehensive exploration of the electronic transport properties of a Janus Ge-based 2D IV-V monolayer. Our investigation employs density functional theory in conjunction with the non-equilibrium Green's function approach. To characterize the current-voltage (I-V) characteristics of the monolayer, we establish a two-probe system with the intrinsic 2D monolayer serving as channel and doped monolayer as electrodes. We systematically investigated the effect of the doping concentration of the probes and channel length on the transport properties. Our results demonstrate that this Janus monolayer displays unique transport characteristics, including a direct bandgap and carrier mobility that depend on the lattice direction, indicating anisotropic transport behavior. These unique characteristics position the monolayer as a promising candidate for applications in the field of nanoelectronics.

HL 7.6 Mon 16:30 ER 325

**Charge Carrier Mobilities in 2D Carbon Allotropes** — •Elif Ünsal[1], Alexander Croy[2], Alessandro Pecchia[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Dresden, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität, Jena, Germany — [3]CNR-ISMN, Monterotondo Stazione, Rome, Italy

Calculation of electron-phonon couplings from first principles is computationally very challenging and remains mostly out of reach particu-

larly for systems with a large number of atoms. Semi-empirical methods, like DFTB, offer a framework to obtain quantitative results at reasonable computational costs. Herein, we are modelling charge transport properties by combining state-of-the-art electron-phonon coupling calculations and semi-classical Boltzmann transport theory. We are using our own code DFTBephy [Croy et al. J. Comput. Electron., 2023] whose implementation is based on DFTB+ [Elstner et al, Phys. Rev. B, 1998] and phonopy [Togo et al, Scr. Mater., 2015] and it interfaces with BoltzTrap2 [Madsen et al., Comput. Phys. Commun., 2018] to calculate transport properties. Our results are bechmarked against state-of-the-art EPW [Poncé et al., Comput. Phys. Comm., 2016] calculations. As a test case, we focused 2D carbon allotropes like graphyne and graphdiyne, and investigated the mechanisms underlying carrier scattering and mobilities within these materials. Our results align with the literature, affirming that the DFTBephy method gives consistent results.

HL 7.7 Mon 16:45 ER 325

**Superconductivity and the normal state quantum geometry in two-dimensional superconductors** — •Florian Simon, Louis Pagot, Marc Gabay, and Mark-Oliver Goerbig — Laboratoire de Physique des Solides, Université Paris-Saclay, Orsay, France

Superconductivity has, since 1911, become a pillar and a flagship of condensed matter physics. The main paradigm is given by BCS theory which, in its standard form, consists of quasiparticles in a single, partially filled band, pairing and thus condensating in a collective dissipationless state. This single band approximation has its limits. Indeed, since the 1980s, physicists have come to realize that in a multiband setting, even adiabatic, each band will carry an influence of the other bands in the form of two geometric quantities, namely the Berry curvature and the quantum metric. These quantities form what we call band/quantum geometry. In the context of superconductivity, this means that even if a single band is involved in the Cooper pairing, it can carry a quantum geometry if the normal state (NS) has more than one band. The influence of this NS quantum geometry on the superconducting state is the subject of this talk. On one side, we study the influence of the NS Berry curvature on BCS theory in the context of two-dimensional massive Dirac fermions. We find that it generally lowers the critical temperature, in a quantifiable way. On another side, we consider the two-dimensional (111) $LaAlO_3/SrTiO_3$ interface. Our results suggest that the quantum metric has a sizeable role in the appearance of superconducting domes in this interface, as a function of gate voltage.

## HL 8: Ultrafast Phenomena I

Time: Monday 15:00–18:00 Location: EW 015

HL 8.1 Mon 15:00 EW 015

**Ultrafast Microbeam Diffraction at 15-keV** — •Johannes Otto[1,2,3], Leon Brauns[1,2], Rudolf Haindl[1,2], Jan Gerrit Horstmann[1,2,4], Armin Feist[1,2], Murat Sivis[1,2], and Claus Ropers[1,2,3] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Max Planck School of Photonics — [4]Present address: Department of Materials, ETH Zürich, Zürich, Switzerland

Ultrafast electron diffraction facilitates the investigation of non-equilibrium structural dynamics [1,2]. In this contribution, we present the development and application of a dedicated setup for microbeam ultrafast electron diffraction ($\mu$-UED), enabling the study of particularly small samples and heterostructures, and promoting experiments on the influence of structural inhomogeneities in non-equilibrium phenomena. We report on the characterization of the spatial and temporal electron beam properties and discuss first time-resolved experiments on a laser-induced structural phase transformation in 1-T tantalum disulfide.

[1] G. Sciaini and R. J. D. Miller, *Rep. Prog. Phys.* **74**, 096101 (2011).

[2] D. Filippetto et al., *Rev. Mod. Phys.* **94**, 045004 (2022).

HL 8.2 Mon 15:15 EW 015

**Time-Domain Coherent Phononics in a Rashba Material** — •Peter Fischer, Julian Bär, Moritz Cimander, Volker Wiechert, Alfred Leitenstorfer, and Davide Bossini — Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany

On the basis of spin-orbit coupling, the emerging research field of spintronics is exploring the possibility of using the spin of electrons instead of their charge as carrier of information. This fundamental interaction also enables the conversion of spin currents into charge currents and vice versa, crucial for linking spintronics and conventional electronics. The Rashba effect, an additional contribution to the spin-orbit coupling in materials lacking inversion symmetry, attracts particular attention in this context. We propose that the excitation of coherent phonons of a specific symmetry has the potential to modulate the bulk Rashba spin-orbit coupling and thus the spin-to-charge conversion efficiency on the ultrashort time scale. In our research, we focus on BiTeI, a layered semiconductor exhibiting a giant bulk Rashba effect. On this material, we perform systematic time-resolved pump-probe measurements of the transient reflectivity. The analysis of the acquired time traces confirms the successful excitation of the targeted coherent phonons at a frequency of 2.7 THz. Tuning the pump-photon energy into the visible, near-infrared and even mid-infrared spectral range, we disclose the most favorable conditions for optical generation of these lattice dynamics and thus, in perspective, for the manipulation of the bulk Rashba spin-orbit coupling.

HL 8.3 Mon 15:30 EW 015

**Light-Induced Nonthermal Phase Transition to the Topological Crystalline Insulator State in SnSe** — •Stefano Mocatti, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Femtosecond pulses have been used to reveal hidden broken symmetry phases and induce transitions to metastable states. However, these states are mostly transient and disappear after laser removal. Photoinduced phase transitions toward crystalline metastable states with a change of topological order are rare and difficult to predict and realize experimentally. In this presentation, by means of constrained density functional perturbation theory and non-perturbative light-induced quantum anharmonicity, we show that ultrafast lasers can permanently transform the topologically trivial orthorhombic structure of SnSe into the topological crystalline insulating rocksalt phase via a first-order nonthermal phase transition (1). We describe the reaction path and evaluate the critical fluence and possible decay channels after photoexcitation. Our simulations of the photoexcited structural and vibrational properties are in excellent agreement with recent pump-probe data in the intermediate fluence regime below the transition, with an error on the curvature of the quantum free energy of the photoexcited state that is smaller than 2%.

(1) S. Mocatti, G. Marini, M. Calandra, J. Phys. Chem. Lett. 2023, 14, 41, 9329-9334

HL 8.4 Mon 15:45 EW 015

**Photoinduced charge density waves in transition metal dichalcogenides** — •Kris Holtgrewe, Giovanni Marini, and Matteo Calandra Buonaura — University of Trento, Italy

Phase transitions induced by ultrafast photoexcitation are an active area of research for materials whose properties can be tuned by light. Transition metal dichalcogenides (TMDs) are a promising class of such materials. Previous studies have demonstrated that photoexcited single layers of $MoTe_2$ and $WTe_2$ show charge density wave (CDW) orders which can be controlled by the photoexcitation strength [1].

In this work, we investigate whether similar phase transitions occur in other 2D TMD homologues, namely $MoS_2$, $WS_2$, $MoSe_2$, and $WSe_2$. Using constrained density functional theory (cDFT) [2], we infer supercell reconstructions from the unstable phonon dispersions of the photoexcited TMDs and analyse their impact on the electronic properties. Our findings reveal that all TMDs undergo a similar CDW-like structural distortion at a material-dependent critical photoexcitation strength. This distortion is characterised by the formation of metal-metal bonds, driven by a charge redistribution between the d orbitals of the metal atoms. Our results provide a comprehensive understanding of the underlying microscopic processes and pave the way for a

general strategy to identify further candidates for photoinduced phase transitions.

[1] G Marini et al. Phys. Rev. Lett. 127, 257401 (2021)
[2] G Marini et al. Phys. Rev. B 104, 144103 (2021)

HL 8.5 Mon 16:00 EW 015

**Polaron Formation Dynamics in BiOI Nanoplatelets Studied by Time-Resolved PEEM** — •Matthias Franz Kestler[1,2], Kyung Chul Woo[2], Justin W. X. Lim[2], Lucas M. Prins[1], Jochen Feldmann[1], and Zhi-Heng Loh[2] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]School of Chemistry, Chemical Engineering and Biotechnology, and School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

BiOI is a nontoxic, stable and polar semiconductor, which shows high conversion efficiencies in photocatalytic water splitting. This is due to an ultrafast and effective charge separation also launching coherent phonons after short laser pulse excitation. The coupling of electronic excitations and phonons should also manifest itself in polaronic effects. To gain unambiguous experimental evidence for polaronic effects we have carried out time-resolved photoemission electron microscopy (TR-PEEM) experiments. This technique offers the unique possibility to learn about the dispersion E(k) of the conduction band (CB) and its occupation with electrons as a function of time after pulsed optical excitation. In order to interpret our data it is not sufficient to describe merely the temporal evolution of the electron distributions in a static CB. We observe that the dispersion of the CB changes itself in time. This is in particular monitored around the Gamma point of the CB. This combined temporal change in band-structure and electron distribution can be explained by the formation of a polaronic excitation.

**15 min. break**

HL 8.6 Mon 16:30 EW 015

**Ultrahigh-Sensitive Optical Detection of Coherent Acoustic Phonons in a GaAs/GaAlAs Superlattice** — •Marek Karzel[1], Anton Samusev[1], Alexey V. Scherbakov[1], Tetiana Linnik[1], Mario Littmann[2], Andrey V. Akimov[3], Dirk Reuter[2], and Manfred Bayer[1] — [1]Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Universität Paderborn, 33098 Paderborn, Germany — [3]University of Nottingham, NG7 2RD Nottingham, United Kingdom

The optical detection of coherent acoustic phonons is a primary tool in ultrafast acoustics. It engages the application of phonons in quantum technology, which is especially promising for nanoscale communications. The ultrahigh-sensitive detection of optically generated phonons with frequencies above 20 GHz can be accomplished due to optical probing in the spectral vicinity of polariton resonance, where a strong permittivity dispersion is observed [1, 2]. In this work, we monitor the propagation of the optically generated coherent phonon wave packet in a semiconductor superlattice of GaAs/$Ga_{0.67}Al_{0.33}As$ at a temperature of 10 K. With the experimental scheme, we achieve a remarkably high detection sensitivity confirmed by probing coherent acoustic wave packets with less than (on average) one phonon within the bandwidth of interest. The lattice strain induced by such a weak elastic perturbation is of an order of $10^{-9}$ with the corresponding lattice displacement of only $\approx 10^{-16}$ m.

[1] A. N. Poddubny, et al., Phys. Rev. B 89, 235313 (2014).
[2] M. Kobecki, et al., Phys. Rev. Lett. 128, 157401 (2022).

HL 8.7 Mon 16:45 EW 015

**Dynamic Observation of Projected Potentials in Switching Semiconductor Diodes by Time-Resolved Electron Holography** — •Tolga Wagner, Hüseyin Çelik, Simon Gaebel, Dirk Berger, and Michael Lehmann — Technische Universität Berlin, Germany

Off-axis electron holography (EH) in a transmission electron microscope (TEM) provides access to nanometer resolved information about the projected electromagnetic potentials of investigated samples. As existing ways for realizing time-resolved measurements in a TEM (e.g. by stroboscopic illumination) have proven to be disadvantageous for EH, such investigations have so far been limited to static measurements.

Recently, a simple, yet promising approach to realize robust time-resolved measurements of periodic processes with nanosecond time resolution in an electron holographic setup by means of interference gating (iGate) was presented. It's based on the synchronized destruction of an interference pattern, relative to an investigated process, where interferometric information is only generated in short undisturbed intervals of a period.

In this presentation, the first application of iGate to switching semiconductor nanostructures, driven at a repetition rate of 3 MHz is demonstrated. By having access to individual frames of the projected electric potential in the area of space charge regions during switching, iGate provides a completely new visual insight into the dynamics of the involved charge carriers with nanometer and nanosecond resolution.

HL 8.8 Mon 17:00 EW 015

**A machine learning approach to non-thermal melting** — •Andrea Corradini, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, via Sommarive 14, 38123 Povo, Italy

Optical laser irradiation of an insulator promotes a fraction of its valence electrons to the conduction band. Often, irradiation transfers electrons from bonding to antibonding states, leading to a weakening of covalent bonds between ion cores. This process is responsible for the insurgence of various non-equilibrium phenomena in photoexcited materials, like non-thermal melting, that occurs when bond weakening is so strong that the crystal structure dissolves and ions rearrange into a new disordered structure. Non-thermal melting on the femtosecond timescale has been observed in photoexcited silicon. Expensive ab initio calculations have also been able to model this process, characterizing its microscopic origin and the resulting disordered structure [1]. Here, we find strong evidence of non-thermal melting in photoexcited silicon by fitting gaussian approximation machine learning potentials to photoexcited equilibrium phases of silicon. Electrons in these phases are treated as a hot Fermi gas for metallic configurations and with the two Fermi level approach for insulating ones [2]. Our findings successfully reproduce most results from real-time time-dependent density functional theory at much lower computational cost and allow us to fully characterize the liquid phases of photoexcited silicon.

[1] Liu, Wen-hao *et al.*. *Sci. Adv.* 8, eabn4430 (2022).
[2] Marini, G. and Calandra, M. *Phys. Rev. B* 104, 144103 (2021)

HL 8.9 Mon 17:15 EW 015

**Molecular dynamics simulations of ultrafast thermodynamics in SrTi03** — •Fredrik Eriksson, Erik Fransson, Richard Matthias Geilhufe, and Paul Erhart — Departement of physics, Chalmers university of technology, Gothenburg, Sweden

The possibility to control and probe materials in the ultrafast regime has opened up several new areas in fundamental research and engineering. In this regard characterization of ultrafast time-dependent thermodynamic properties within the material is crucial [1]. Here, we analyze these aspects by molecular dynamics for the cubic perovskite SrTi03. In particular we artificially excite the ferroelectric optical phonon mode at the zone center, mimicking a laser response. The mode interactions and decay pathways are analyzed and compared to theoretical and experimental data. We find that after about 500fs of pumping the ferroelectric mode, a higher frequency optical mode at Gamma, around 6THz, is strongly excited and pushed out of its equilibrium distribution. This observation is in good agreement with recent experimental work using time-resolved X-ray scattering where this upconversion was also observed [2]. The method allows for a detailed understanding of the entropy production in the system from first principles. In addition, the microscopic mechanism responsible for the upconversion are outlined.

[1] Caprini et al. arXiv:2302.02716v2 (2022)
[2] Kozina et al. Nat. Phys. 15, 387-392 (2019)

HL 8.10 Mon 17:30 EW 015

**Ultrafast Nanobeam Electron Diffraction of Charge-Density Wave Phase Transitions at Megahertz Rates** — •Till Domröse[1,2] and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Ultrafast electron diffraction (UED) is capable of unveiling ultrafast structural dynamics in functional materials [1]. Its intrinsic spatial averaging, however, limits the characterization of nanoscale heterogeneity, which often decisively influences the dynamics, or even is a source of functionality itself. Here, we demonstrate how the high-coherence electron source of the Göttingen Ultrafast Transmission Electron Microscope (UTEM) [2] enables the formation of highly collimated,

nanometer-sized, femtosecond electron pulses for UED. We investigate laser-induced charge-density wave dynamics in the strongly-correlated materials 1$T$-$TaS_2$ and 1$T$-$TaTe_2$ at an unprecedented repetition rate of up to 2 MHz. Therein, the high reciprocal-space resolution allows us to identify a light-induced hexatic state via a three-dimensional characterization of transient disorder [3]. Furthermore, the significant signal enhancement in combination with the small probe volume facilitates access to laser-induced phase transitions with high sensitivity, paving the way for the investigation of non-equilibrium structural dynamics in heterogeneous systems on their intrinsic timescales.

[1] D. Filippetto *et al.*, Rev. Mod. Phys. **94**, 045004 (2022)
[2] A. Feist *et al.*, Ultramicroscopy **176**, 63-73 (2017)
[3] T. Domröse *et al.*, Nat. Mater. **22**, 1345-1351 (2023)

HL 8.11 Mon 17:45 EW 015

**Institute of Physics, Rostock University, 18051 Rostock, Germany** — •Siamak Pooyan and Dieter Bauer — Institute of Physics, Rostock University, 18051 Rostock, Germany

It has been found previously that the presence or absence of topological edge states in the Su-Schrieffer-Heeger (SSH) model in its topological and trivial phase, respectively, has a huge impact on harmonic generation spectra. More specifically, the yield of harmonics for harmonic orders that correspond to photon energies below the band gap is many orders of magnitude different in the trivial and topological phase. It is shown in this work that this effect is still present if nearest-neighbor electron-electron interaction is taken into account, i.e., if a Hubbard term is added to the SSH Hamiltonian. To that end, finite SSH-Hubbard chains at half filling are considered that are short enough to be accessible to exact diagonalization but already showing edge states in the topological phase. We show that the huge difference in the harmonic yield between trivial and topological phase can be reproduced with few-level models employing only the many-body ground state and a few excited many-body states in the trivial and topological phase, respectively.

## HL 9: 2D Materials and Heterostructures: Interlayer Excitons

Time: Monday 15:00–18:30 Location: EW 201

HL 9.1 Mon 15:00 EW 201

**New interlayer excitons in 2D bilayers revealed under strong electric field** — •Sviatoslav Kovalchuk[1], Kyrylo Greben[1], Abhijeet Kumar[1], Simon Pessel[1], Jan Soyka[2], Qing Cao[2], Kenji Watanabe[3], Takashi Taniguchi[3], Dominik Christiansen[4], Malte Selig[4], Andreas Knorr[4], Siegfried Eigler[2], and Kirill Bolotin[1] — [1]Physics Department, FU Berlin, Berlin — [2]Institute of Chemistry and Biochemistry, FU Berlin, Berlin — [3]National Institute for Materials Science, Tsukuba, Japan — [4]Physics Department, TU Berlin, Berlin

Excitons in bilayer transition metal dichalcogenides (2L-TMDs) are Coulomb-bound electron/hole pairs that can be viewed as broadly tunable analogs of atomic or molecular systems. Here, we study the properties of 2L-TMD excitons under a strong electric field. To overcome the field limit reached in previous experiments, we developed a new organic/inorganic molecular gating technique. This approach allows us to achieve an electric field strength of about 0.35 V/nm, more than a factor of two higher than achieved previously in purely solid-state gated devices. Under this field, inter- and intralayer excitons are brought into an energetic resonance, allowing us to discover new emergent properties of the resulting states. We detect a previously unseen interlayer exciton that only becomes visible at high field through hybridization with A exciton. Moreover, the system experiences an ultra-strong Stark splitting of $>$ 380 meV with exciton energies tunable over a large range of the optical spectrum, holding potential for optoelectronics.

HL 9.2 Mon 15:15 EW 201

**Signatures of efficient intervalley scattering by acoustic phonons in WSe2/MoSe2 heterostructure** — •Hendrik Lambers[1], Nihit Saigal[1], Jonas Kiemle[2], Alexander W. Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Germany

The ability to host excitonic phenomena and correlated phases gives rise to many recent studies on TMDC bilayers. In particular interlayer excitons in heterobilayers are promising candidates to form coherent many body states [1]. The role of exciton-phonon interaction for the thermalization process of these interlayer excitons and the dominant type of involved phonons are of ongoing interest [2]. We employ resonant Raman scattering at cryogenic temperatures to study the exciton phonon coupling in WSe2/MoSe2 heterostructures. The resonance profiles of degenerated WSe2 A1'/E' phonon modes are significantly affected by the assembly into heterobilayers. The profiles cannot be explained only by an incoming and an outgoing resonance of a first order Raman process. Our findings indicate a higher order Raman scattering process involving acoustic M or K point phonons of WSe2 and therefore strong interaction of acoustic phonons with electronic states, that results in efficient intervalley scattering of charge carriers. [1] M. Troue et al., Phys. Rev. Lett. 131, 036902 (2023). [2] M. Katzer et al., Phys. Rev B 108, L121102 (2023).

HL 9.3 Mon 15:30 EW 201

**Emergent Trion-Phonon Coupling in Atomically Reconstructed $MoSe_2$-$WSe_2$ Heterobilayers** — •P. Parzefall[1], S. Meier[1], Y. Zhumagulov[2], M. Dietl[1], N. Meier[1], J. Lichtenberger[1], M. Kempf[1], J. Holler[1], P. Nagler[1], K. Watanabe[3], T. Taniguchi[3], P. E. Faria JR.[2], J. Fabian[2], T. Korn[4], and C. Schüller[1] — [1]Institut für Exp. und Angewandte Physik, Uni Regensburg (UR), Germany — [2]Institut für Theo. Physik, UR, Germany — [3]NIMS, Tsukuba Ibaraki, Japan — [4]Institut für Physik, Uni Rostock, Germany

We report about low-frequency Raman studies on atomically-reconstructed $MoSe_2$-$WSe_2$ heterostructures (HS) at cryogenic temperatures. In these experiments, we tune a Ti:Sapphire laser into close resonance to the intralayer excitonic transitions of both, $MoSe_2$ and $WSe_2$, and compare the resulting Raman spectra to the well-known off-resonant case [1]. We detect a low-enery Raman mode, which is observable only at the intralayer trion ($X^-$) resonances. The energy of the emergent Raman mode is close to the interlayer shear mode (ISM) of the HS [1] but it exhibits different polarization selection rules and a lineshape, resembling a Fano-profile.
We interpret our results as follows: The $X^-$ gains an interlayer character via its second electron, which is located in the Q valley and distributed over both layers, and which enables the coupling to the interlayer shear mode. [1] J. Holler et al., APL **117**, 013104 (2020) [2] S. Meier et al., Phys. Rev. Res. **5**, L032036 (2023)

HL 9.4 Mon 15:45 EW 201

**Spin Relaxation of Interlayer Excitons in TMDC Heterostructures** — •Henry Mittenzwey[1], Abhijeet Kumar[2], Kirill Bolotin[2], Malte Selig[1], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

TMDC heterobilayers are promising candidates for new excitonic phases, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different atomically thin layers. The relaxation dynamics of these interlayer excitons after their optical excitation is still under investigation.

Based on Heisenberg equations of motion and a correlation expansion of many-body interactions, we discuss the temporally resolved spin dynamics of interlayer excitonic occupations in momentum space: Due to charge separation, interlayer excitons give rise to an out-of-plane self-induced electric field. This leads to Rashba spin-orbit interaction, which is absent in TMDC monolayers. By tuning the total excitonic interlayer occupation, the strength of the internal electric field can be varied and the Rashba spin relaxation can be enhanced or suppressed.

To address the experimental verification of these effects, we discuss, how spin relaxation dynamics of interlayer excitons can be detected in optical pump probe measurements.

HL 9.5 Mon 16:00 EW 201

**Impact of hybrid exciton-exciton interactions on transport in 2D materials** — •Daniel Erkensten[1], Samuel Brem[2], Raul Perea-Causin[1], Joakim Hagel[1], Fedele Tagarelli[3], Edoardo Lopriore[3], Ermin Malic[2,1], and Andras Kis[3] — [1]Chalmers University of Technology — [2]Philipps-Universität Marburg — [3]Ecole Polytechnique Fédérale de Lausanne

Transition-metal dichalcogenide bilayers host exciton states that hybridize via electron or hole tunneling, forming layer-hybridized excitons with large oscillator strengths and out-of-plane dipole moments. In this joint theory-experiment work, we combine microscopic many-particle theory with spatiotemporal measurements to investigate the role of hybrid exciton-exciton interactions in exciton transport in $WSe_2$ homobilayers [1,2]. The energetically lowest state in these structures is shown to be electrically tunable, transitioning from an intralayer-like to an interlayer-like ground state via the application of an out-of-plane electric field [1]. This finding leads to two intriguing interaction regimes for hybrid excitons: a low-dipole regime at small electric fields involving weakly interacting excitons which exhibit conventional diffusion, and a high-dipole regime at elevated electric fields governed by strongly interacting excitons and highly anomalous diffusion. Our work highlights the remarkable electrical tunability of hybrid exciton-exciton interactions, providing insights for future research in this evolving field.

[1] D.Erkensten et al. Nanoscale, 15, 11064-11071 (2023).
[2] F. Tagarelli, D. Erkensten et al. Nat. Photonics, 71, 615-621 (2023).

HL 9.6 Mon 16:15 EW 201

**Manipulation of hybrid interlayer excitons in 2D materials** — •M. Federolf, A. Davgol, E. Flanagan, M. Emmerling, V. Kaushik, and S. Höfling — Julius-Maximilians-Universität Würzburg, Lehrstuhl für Technische Physik

It has been shown, that in two layers of transition-metal dichalcogenides hybrid interlayer exciton can form by the coupling of the interlayer exciton with the intralayer exciton [1]. Here the electron in one layer interacts with a tunneling hole located betwen the layers. This configuration exhibits an out of plane dipole moment while maintaining a large oscillator strength due to the hybrid character. The degeneration of the dipole orientation can be lifted using an external electric field leading to a splitting into two distinct states [2,3].

Further, these hybrid interlayer excitons promise enhanced interaction with themselves compared to the A exciton. By introducing a higher density, the blueshift of the hybrid interlayer polaritons exceeds the blueshift of the A polaritons [4,5].

We try to combine those effects by introducing higher exciton densities while simultaneously applying an out of plane electric field and investigating the interaction of the different excitons.

References [1] Gerber, I.C., et al. Phys. Rev. B 99, 035443 (2019). [2] Lorchat, E., et al., Phys. Rev. Lett. 126, 037401 (2021). [3] Leisgang, N., et al., Nat Nano 15, 901*907 (2020). [4] Datta, B., et al., Nat Comm 13, 6341 (2022). [5] Louca, C., et al., Nat Comm 14, 3818 (2023).

**15 min. break**

HL 9.7 Mon 16:45 EW 201

**Extended spatial coherence of interlayer excitons in $MoSe_2/WSe_2$ heterobilayers** — •Johannes Figueiredo[1,2], Mirco Troue[1,2], Lukas Sigl[1,2], Christos Paspalides[1,2], Manuel Katzer[3], Malte Selig[3], Andreas Knorr[3], Ursula Wurstbauer[4], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]MCQST — [3]Institute for Theoretical Physics, Nonlinear Optics and Quantum Electronics, TU Berlin — [4]Institute of Physics, Münster University

A heterobilayer arrangement of $MoSe_2/WSe_2$ monolayers allows the optical generation of long-lived electron-hole pairs known as interlayer excitons [1]. Consequently, those heterostructures present an ideal platform to study optically excited many-body phenomena of an interacting Bose gas at low bath temperatures [2]. Our work advances the study of coherent, photoluminescent interlayer exciton ensembles in $MoSe_2/WSe_2$ heterobilayers by utilizing a spatially resolved point-inversion Michelson-Morley interferometer. We report on the spatial coherence of a dense interlayer exciton ensemble for a wide range of temperatures and exciton densities. Below 10 K, we detect a spatial coherence length of interlayer excitons limited only by the lateral expansion of the exciton ensembles. Our research sheds new light on the physics of coherent exciton phases in the proposed heterostacks [3].

[1] L. Sigl *et al.*, Phys. Rev. Research 2, 042044(R) (2020) [2] M. Katzer *et al.*, Phys. Rev. B 108, L121102 (2023) [3] M. Troue and J. Figueiredo *et al.*, Phys. Rev. Lett. 131, 036902 (2023)

HL 9.8 Mon 17:00 EW 201

**Theory of interlayer excitons dynamics in 2D TMDCs Heterolayers including reconstruction through strain and disorder** — •Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

After combining two TMDC monolayers to form a heterolayer small angles between the lattices lead to the formation of Moiré structures.

Recently it has been shown, that strain leads to a reconstruction of the domains formed by the Moiré structure. This contribution uses reconstructed strain fields with some disorder as a basis to calculate the potential landscape of electrons and holes forming interlayer excitons.

Opposed to the common solution of the center-of-mass exciton wave function in reciprocal space, here the wave function is solved in real space to accommodate disorder and to provide additional insights into the structure of exciton states. Using the obtained exciton basis exciton-phonon scattering elements and lineshapes are calculated after a polaron transformation, which allows the calculation of exciton relaxation and realistic optical signals such as linear absorption, PL.

HL 9.9 Mon 17:15 EW 201

**The impact of twist angle and band alignment on the excitation of valley-polarized free charge carriers in WSe2/MoSe2 heterobilayers** — •Jo Bertram[1], Marc Schütte[1], Frank Volmer[2], Manfred Ersfeld[1], Lars Rathmann[1], Kenji Watanabe[3], Takashi Taniguchi[4], Christoph Stampfer[1], Lutz Waldecker[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Germany — [2]AMO GmbH, Advanced Microelectronic Center Aachen (AMICA), Aachen, Germany — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

Transition metal dichalcogenides (TMDs) are of interest in valley- and spintronics due to the fact that a valley polarization in these materials can be created by circularly polarized light [1]. Here, we show that the band alignment in heterostructures of different TMD monolayers enables new ways of transferring the valley polarization between the layers. In particular, we identify a transfer process in WSe2/MoSe2 heterostructures where the polarization from excitons in WSe2 is transferred to free charge carriers in MoSe2, exhibiting valley lifetimes that are strongly dependent on the twist angle [2]. Furthermore, we show that a variation in the doping of the TMDs as well as the addition of an hBN spacer layer significantly impacts the band alignment of the heterostructure, resulting in fundamentally different valley dynamics.

[1] Nature Reviews Materials 7, 449 (2022), [2] npj 2D Mater Appl 7, 58 (2023)

HL 9.10 Mon 17:30 EW 201

**Investigating moiré interlayer excitons under the influence of atomic reconstructions** — •Nils-Erik Schütte[1], Carl Emil Mørch Nielsen[2], Niclas Götting[1], Frederik Lohof[1], Gabriel Bester[2], and Christopher Gies[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Institute of Physical Chemistry, University of Hamburg

The moiré pattern which emerges due to a relative rotation between two monolayers of transition metal dichalcogenides (TMDs) features a long lattice period for small twist angles. The resulting band structure modulation acts as an effective potential for interlayer excitons (IXs). However, lattice reconstructions change the moiré potential which forms broader and deeper potential minima, realizing a periodic array of quantum wells for IXs. This serves as an implementation of the Bose-Hubbard (BH) model for the simulation of correlated excitonic states.

Expanding on previous results [1], we describe the correlated behavior of IXs in the moiré lattice with an extended BH model taking into account non-local interactions and a material realistic modelling of the dielectric screening. Considering interatomic forces, we discuss how the BH parameters and especially the excitonic wave functions are influenced by local atomic reconstructions. Furthermore, by solving the BH model with a sublattice mean-field description, we address the question in how far correlated states of moiré excitons emerge at different twist angles and integer as well as fractional lattice fillings.

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

HL 9.11 Mon 17:45 EW 201

**Pressure Dependence of Intra- and Interlayer Excitons in 2H-$MoS_2$ Bilayers** — •Jan-Hauke Graalmann[1], Paul Steeger[2], Robert Schmidt[2], Ilya Kupenko[3], Carmen Sanchez-Valle[3], Philipp Marauhn[1], Thorsten Deilmann[1], Steffen Michaelis de Vasconcellos[2], Michael Rohlfing[1], and Rudolf Bratschitsch[2] — [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 — [3]University of Münster, Institute of Mineralogy, Corrensstr. 24, 48149 Münster

The optical spectrum of the $MoS_2$ bilayer changes under pressure as theoretical and experimental studies have shown [1].

Our computational investigations of the structural, electronic and optical properties are based on elasticity theory, DFT, *GdW* and the Bethe-Salpeter equation. The stress conditions in our diamond anvil cell experiment result in an effective shift of the excitation energy of the A exciton towards higher energies with increasing pressure. This shift corresponds strongly to the behavior of the direct band gap at the K point. Due to a growing valence band splitting for increasing pressures, the interlayer exciton shows a smaller shift. In total, the A-IL energy splitting decreases under pressure.

Furthermore, the theoretical reproduction of the experimental results shows a suppression of the transfer of hydrostatic pressure due to the interaction between the bilayer and the substrate.

[1] P. Steeger, J.-H. Graalmann et al., Nano Lett., 23, (2023)

HL 9.12 Mon 18:00 EW 201

**Correlated Magnetism in Moiré Exciton-Polaritons** — •Lukas Lackner[1], Johannes Scherzer[2], Bo Han[1], Jens-Christian Drawer[1], Christoph Bennenhei[1], Martin Esmann[1], Alexander Högele[2], and Christian Schneider[1] — [1]Carl von Ossietzky University Oldenburg, Germany — [2]Ludwig-Maximilians-Universität München, Germany

Due to the reduced dielectric screening in van der Waals materials, Coulomb interactions and many-body correlations are enhanced. This allows for a large variety of experimentally observables such as Wigner crystals, quantum Hall phases and Hubbard-correlated magnetic phases. In Moiré lattices, due to the periodic potential landscape and thus the reduced kinetic energy of confined quasi-particles, correlations display their fingerprints more prominently. In this work, we present the evolution of a correlation induced magnetic phase of Moiré confined exciton-polaritons based on a charge tunable MoSe2/WS2 van der Waals heterostructure in a spectrally tunable open microcavity. Approaching the Mott state of the triangular Moiré lattice at a filling of one electron per lattice site, Moiré exciton-polartions acquire a giant, nonlinear g-factor reflecting the emergence of correlated magnetism in our electron system.

HL 9.13 Mon 18:15 EW 201

**Theoretical description of ultraviolet interlayer trions in bilayer 2H-$WSe_2$** — •Ruven Hübner[1], Alexander Steinhoff[1], and Matthias Florian[2] — [1]Institut für Theoretische Physik, Universität Bremen, Germany — [2]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

For an extended period, interlayer excitons in bilayers of transition metal dichalcogenides (TMDs) have received a great deal of attention. Numerous studies have explored the influence of material combination, stacking configuration, twist angle and external electric fields. However, most such studies exclusively focus on excitons, formed near the band edge, confined to electronic states with a parabolic dispersion and a homogeneous interlayer character. More recently, experimental findings have unveiled ultraviolet excitons, involving high-lying and non-parabolic bands of TMD materials at approximately double the band gap energy [1]. These states open up the possibility of forming new kinds of trions, in which the additional charge carrier is provided by doping electrons near the band edge. In this talk we focus on such high-lying trions formed within a $WSe_2$ inversion symmetric homobilayer. We develop a theoretic framework, which classifies distinct trion species based on their dominant interlayer localization of each of the three constituent particles, starting from Wannierized electronic states based on a DFT calculation. We discuss the influence of doping density and use our results to explain very recent experiments.

[1] KQ. Lin et al., Nature Communications **12**, 5500 (2021)

## HL 10: Focus Session: Evolution of Topological Materials into Superconducting Nanodevices I (joint session HL/TT)

The focus session intends to span the arc between topological materials and superconducting nanodevices, both experimentally and theoretically. Such structures are interesting for applications in future topological quantum circuits. In recent years, the number of topological materials and the knowledge about them has rapidly increased. As part of the focus session, material properties of layered systems made of topological materials, especially in combination with superconductors, are discussed. On the other hand, the special challenges in the nanofabrication of these materials for use in future topological quantum processors are addressed. Another focus is the quantum transport in nanoscale hybrid structures.

Organized by Thomas Schäpers, Philipp Rüßmann, and Peter Schüffelgen

Time: Monday 15:00–18:00 Location: EW 202

HL 10.1 Mon 15:00 EW 202

**Transport studies in selectively grown topological insulator multiterminal Josphson junctions** — •Gerrit Behner[1,2], Alina Rupp[1,2], Abdur Rehman Jalil[1,2], Kristof Moors[1,2], Dennis Heffels[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jara-Fundamentals of Future Information Technology, Forschungszentrum Jülich and RWTH Aachen University, Germany

The combination of an ordinary s-type superconductor with three-dimensional topological insulators creates a promising platform for fault tolerant topological quantum computing circuits based on Majorana braiding. The backbone of the braiding mechanism are three terminal Josephson junctions. It is crucial to understand the transport in these devices for further use in quantum computing applications. We present low-temperature measurements of three-terminal $Bi_{0.8}Sb_{1.2}Te_3$ Josephson junctions fabricated, based on a combination of selective area growth and shadow mask evaporation. The transport properties of the junction are mapped out as a function of bias current and magnetic field. The bias current maps reveal a variety of transport phenomena, i.e. multiple Andreev reflections suggesting the successful fabrication of a fully coupled three-terminal junction. The junctions seem to be in good agreement with a resistively and capacitively shunted junction model, but also reveal the influence of intrinsic asymmetries and their effect on the transport in the junctions.

HL 10.2 Mon 15:15 EW 202

**Quasparticle poisoning effects on electron transport through a Majorana wire** — •Florinda Viñas Boström[1,2] and Patrik Recher[1,3] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Division of Solid State Physics and NanoLund, Lund University, Box 118, S-221 00 Lund, Sweden — [3]Laboratory of Emerging Nanometrology, D-38106 Braunschweig, Germany

Majorana bound states have been suggested as building blocks for fault-tolerant quantum computational devices. However, a problem

for both Majorana based and other types of superconducting qubits, is quasi-particle poisoning, where an additional quasiparticle changes the parity of the superconducting condensate. In this work, we show how quasi-particle poisoning affects electron transport through a Majorana wire coupled to current leads on each side of the wire, using an open systems approach combining master equations with full counting statistics. To describe the correct low-energy physics for current and noise, we include sequential- and co-tunneling processes in our description. We believe that our study will be a guide both for future theoretical work, and to analyze transport experiments of such setups.

HL 10.3 Mon 15:30 EW 202

**Andreev spectrum of Josephson junctions with topological insulator nanostructures** — •Dennis Heffels, Peter Schüffelgen, Kristof Moors, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany

Josephson junctions and the presence of Andreev bound states play an important role in quantum information and quantum materials research, forming an integral part of SQUIDs and superconducting qubits, for example. The bound states within a Josephson junction have a phase-dependent spectrum known as the Andreev spectrum. The investigation of this spectrum with phase-sensitive measurements can be used to characterize exotic types of superconductivity, such as topological superconductors with Majorana bound states. Here we present a method to efficiently calculate numerically detailed Andreev spectra, based on a scattering matrix method and (3D) tight binding, for different junction geometries, chemical potential and disorder profiles, etc. We apply this method to proximitized topological insulator (TI) nanostructure-based junctions in which Majorana bound states are expected upon application of an external magnetic field. In this setup, the spin-momentum-locked topological surface states give rise to highly unconventional Andreev spectra and corresponding current-phase relationships, both in the topologically trivial and nontrivial superconducting regimes.

HL 10.4 Mon 15:45 EW 202

**Realistic modeling of proximitized magnetic topological insulator nanoribbons** — •Eduárd Zsurka[1,2,3], Julian Legendre[3], Daniele Di Miceli[3,4], Llorenç Serra[4], Thomas Schmidt[3], and Kristof Moors[1,2] — [1]PGI-9, Forschungszentrum Jülich — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University — [3]Department of Physics and Materials Science, University of Luxembourg — [4]Department of Physics, University of the Balearic Islands

Proximitized magnetic topological insulator nanoribbons (PMTINRs) are a potential platform for the practical realization of the Majorana zero-energy mode (MZM) [1]. Here, we present a realistic description of PMTINRs and similar superconductor-topological insulator heterostructures. Both bulk and effective surface-state models are used to capture the low-energy electronic spectrum, with realistic parameters extracted from *ab initio* calculations. Using numerical simulations, we study in a tight-binding framework the properties of PMTINRs. Particular attention is given to the thin-film limit, where theoretical results have been conflicting on the topology of the hybridization gap. Magnetic and nonmagnetic disorder, as well as device imperfections, can all be detrimental to the formation of MZMs in PMTINRs. We aim to clarify what are the optimal conditions to obtain MZMs in PMTINRs, that are robust against such effects.

[1] C.-Z. Chen, Y.-M. Xie, J. Liu, P. A. Lee, and K. T. Law, Phys. Rev. B 97, 104504 (2018).

HL 10.5 Mon 16:00 EW 202

**Transport in core/shell GaAs/InAs/Al half-shell nanowire-based hybrid devices** — •Farah Basarić[1,2], Patrick Zellekens[3], Russell Deacon[3], Vladan Brajović[1,2], Alexander Pawlis[1,2], Gerrit Behner[1,2], Hans Lüth[1,2], Detlev Grützmacher[1,2], Koji Ishibashi[3], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]RIKEN Center for Emergent Matter Science and Advanced Device Laboratory, 351-0198 Saitama, Japan

Epitaxially grown core-shell GaAs/InAs nanowires provide a heterostructure with transport properties governed by the angular momentum states in the InAs shell. Besides conventional polymorphic GaAs/InAs nanowires, phase-pure core/shell nanowires featuring only wurtzite crystal structure along the axis were studied by magnetotransport measurements under an axial magnetic field. Transport regime analysis for both nanowire types indicates the presence of Aharonov-Bohm-type oscillations, while magnetotransport analysis suggests a strong effect of disorder reduction for phase-pure nanowires. This is manifested by the presence of the quasi-ballistic transport regime, indicating superior transport properties of the phase-pure nanowire. Combining phase-pure GaAs/InAs nanowires with an in-situ deposited superconducting Al half-shell, a gate-controlled Josephson junction was fabricated.

HL 10.6 Mon 16:15 EW 202

**Van der Pauw measurements for the optimization of magnetic topological insulators** — •Jan Kartheiner[1,3], Jonas Buchhorn[1,3], Kaycee Underwood[1,3], Abdur Reman Jalil[1,3], Peter Schüffelgen[1,3], Detlev Grützmacher[1,2,3], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Peter Grünberg Institut (PGI-10), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany

Quantum anomalous Hall insulators are proposed to be a platform for the realization of chiral Majorana edge modes when coupled to a superconductor by the proximity effect. The quantum anomalous Hall state has already been achieved in magnetic topological insulators but inducing superconductivity into these materials remains a challenge. We present a measurement scheme based on the van der Pauw method that allows to get fast insights into the electrical transport properties of thin films at low temperatures prepared by molecular beam epitaxy. On the example of Cr-doped $(Bi_xSb_{1-x})_2Te_3$ the effect of different growth parameters is investigated and compared to Hall bar measurements. The van der Pauw method enables a fast feedback loop between growth and transport measurements. This will help to establish a reliable epitaxial growth of quantum anomalous Hall insulator thin films and allow to systematically search for promising material compositions to induce superconductivity into magnetic topological insulators.

**15 min. break**

HL 10.7 Mon 16:45 EW 202

**Topology of finite size magnetic topological insulator/superconductor heterostructures** — •Julian Legendre[1], Eduárd Zsurka[1,2,3], Daniele Di Miceli[1,4], Llorenç Serra[4,5], Kristof Moors[2,3], and Thomas L. Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg — [2]PGI-9, Forschungszentrum Jülich — [3]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University — [4]Institute for Cross-Disciplinary Physics and Complex Systems IFISC (CSIC-UIB) — [5]Department of Physics, University of the Balearic Islands

Heterostructures of magnetic topological insulators (MTIs) and superconductors (SCs) in two-dimensional (2D) slab and one-dimensional (1D) nanoribbon geometries have been predicted to host chiral Majorana edge states or Majorana bound states (MBS), respectively. We study the topological properties of such MTI/SC heterostructures upon variation of the slab geometry from wide slabs to quasi-1D nanoribbon systems and as a function of the chemical potential, the magnetic doping, and the induced superconducting pairing potential. To do so, we construct effective symmetry-constrained low-energy $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians accounting for the real-space confinement. Transitions between topological phases are then signalled by sign changes of the resulting gap magnitude at the $\Gamma$ point. For confined slab geometries, as the chemical potential, the magnetic doping and/or the width of the slab are varied, we observe a periodic sign change of the bulk gap, which entails reentrant MBS at the ends of the nanoribbon.

HL 10.8 Mon 17:00 EW 202

**Proximity induced superconducting gap in Bi-containing thin TI and highly ordered TI films grown on the Nb(110) surface** — •Artem Odobesko, Felix Friedrich, Robin Boshuis, and Matthias Bode — Julius-Maximilians-Universität Würzburg,Physikalisches Institut, Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany

A superconductor (SC) in contact with a non-SC metal leads to a prox-

imity effect, wherein Cooper pairs from the SC infiltrate the metal. The proximity effect has recently regained attention due to its potential for achieving topological superconductivity within heterostructures of 3D topological insulators (TI) combined with conventional s-wave SC. Theoretical predictions suggest the emergence of Majorana zero-energy modes within the vortices of such TI/SC heterostructures. The magnitude of the proximity-induced gap is pivotal for the robustness of Majorana zero modes and in general distinct from proximity pairing correlations. The current experiments are aimed at examining the induced SC-gap on the exposed surface of thin Bi-containing slabs -Bi(111), Bi(110) and $Bi_2Te_3$ - grown on Nb(110) substrate. The characteristics of the induced SC-gap are not solely dependent on the thickness of the slab; they are also strongly influenced by the matching of Fermi surfaces between the SC and non-SC materials at their interfaces. The band structure correspondence and band bending at the interface, plays a crucial role in generating a robust proximity-induced SC-gap. It underscores the necessity to explore compatible pairs of SC and non-SC materials for effective band matching.

HL 10.9 Mon 17:15 EW 202

**Selective growth of magnetic topological insulator nanostructures via molecular beam epitaxy** — •Max Vassen-Carl, Peter Schüffelgen, and Detlev Grützmacher — Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany

Magnetic topological insulators (MTIs) have great potential for hosting Majorana zero modes [1]. To achieve this, MTI nanostructures are a promising candidate. In such devices, the chiral edge modes (CEM) of the MTI are predicted to hybridise [2]. To verify this prediction, other groups have etched MTI films into thin Hallbars [3]. This etching process is prone to damage the edge states.
In this work a new molecular beam epitaxy (MBE) technique is presented, which enables the selective growth of MTI structures for the first time. Transport measurements on such devices provide insights into the size dependence of CEM in MTIs.

[1] D. Burke et al., arXiv 2302.10982 (2023)
[2] Chen et al., Phys. Rev. B 97, 104504 (2018)
[3] Zhou et al., Phys. Rev. Lett. 130, 086201 (2023)

HL 10.10 Mon 17:30 EW 202

**Conductance asymmetry in proximitized magnetic topological insulator junctions with Majorana modes** — •Daniele Di Miceli[1,2], Eduárd Zsurka[2,3,4], Julian Legendre[2], Kristof Moors[3,4], Thomas Schmidt[2], and Llorenç Serra[1,5] — [1]Institute for Cross-Disciplinary Physics and Complex Systems IFISC (CSIC-UIB) — [2]Department of Physics and Materials Science, University of Luxembourg, 1511 Luxembourg, Luxembourg — [3]PGI-9, Forschungszentrum Jülich — [4]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University — [5]Department of Physics, University of the Balearic Islands

Magnetic topological insulators are outstanding candidates for the realization of topological 1D and 2D superconducting phases when coupled by proximity to ordinary *s*-wave superconductors. We study normal-superconductor-normal junctions made of narrow (wirelike) or wide (filmlike) magnetic topological insulator slabs with a central proximitized sector. Specifically, we investigate how the electronic transport depends on the topological phase of the central superconductor when the voltage bias is split asymmetrically between the two normal leads of the junction. The occurrence of charge-nonconserving Andreev processes entails a nonzero conductance related to an electric current flowing to ground from the proximitized sector of the junction. We show that topologically protected Majorana modes require an antisymmetry of this conductance with respect to the point of equally split bias across the junction.

HL 10.11 Mon 17:45 EW 202

**Transport spectroscopy on $(Bi,Sb)_2Te_3$ nanoribbons proximitized by aluminum as parent superconductor** — •Benedikt Frohn, Tobias W. Schmitt, Vanessa S. Bello, Dennis Heffels, Albert Hertel, Michael Schleenvoigt, Abdur R. Jalil, Kristof Moors, Peter Schüffelgen, and Detlev Grützmacher — Peter Grünberg Institut, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, D-52425 Jülich, Deutschland

One-dimensional topological insulator nanowires which are proximitized by an s-wave superconductor and are exposed to an in-plane magnetic field are predicted to become topological superconductors [1, 2]. So far, realizing a strong proximity effect in such structures has remained an experimental challenge. In this talk, I present transport spectroscopy results on $(Bi,Sb)_2Te_3$ nanowires with Al as parent superconductor. All materials are grown via molecular beam epitaxy in a single growth run consisting of six subsequent deposition steps. To prevent diffusion of Al into $(Bi,Sb)_2Te_3$ and creating a transparent interface, we employ a thin diffusion barrier made from Pt. These devices are fabricated using stencil lithography [3] and possess contacts with varying barrier strength made of AlOx. This enables us to study the density of states and therefore to search for topological features within the induced superconducting gap, of which we measure the dependences of different magnetic field directions as well as temperature.

[1] Cook et al., Phys. Rev. B 86, 155431 (2012)
[2] Heffels et al., Nanomaterials 13, 723 (2023)
[3] Schüffelgen et al., Nat. Nanotechnology 14, 825-831 (2019)

## HL 11: Materials and Devices for Quantum Technology I (joint session HL/QI)

Time: Monday 15:00–18:00 Location: EW 203

HL 11.1 Mon 15:00 EW 203

**A Quantum Polyspectra Approach to the Analysis of Quantum Emitter Blinking Dynamics at Low Photon Rates Without Binning** — •M. Sifft[1], A. Kurzmann[2], J. Kerski[4], R. Schott[3], A. Ludwig[1], A. D. Wieck[1], A. Lorke[4], M. Geller[4], and D. Hägele[1] — [1]Ruhr Uni., DE — [2]RWTH Aachen, DE — [3]ETH Zürich, CH — [4]Uni. Duisburg-Essen, DE

The statistical analysis of quantum emitters becomes hard or even impossible for traditional methods like the full counting statistics in cases of decreasing light levels. We propose a polyspectra approach that prevails even in scenarios of high photon losses or low photon rates. A minimum photon flux and binning of photon-events is no longer required [1]. By comparing theoretical polyspectra (higher-order generalizations of the usual power spectrum) with those calculated directly from the detector output, we can identify the emitter's Liouvillian or transition matrix.

We analyze quantum dot fluorescence data and determine on-off switching rates at average photon rates much lower than the system dynamics. Our Python libraries, SignalSnap and QuantumCatch, are freely available for computing polyspectra on GPUs and for their subsequent analysis [2,3]. The libraries allow for an advanced analysis of general continuous quantum measurements yielding the systems Liouvillian or its underlying hidden Markov model.

[1] Sifft et al., arXiv:2310.10464,
[2] github.com/markussifft/signalsnap,
[3] github.com/markussifft/quantumcatch

HL 11.2 Mon 15:15 EW 203

**A type-IV gatemon qubit based on Ge/Si core-shell nanowires** — Han Zheng[1], Luk Yi Cheung[1], Nikunj Sangwan[1], Roy Haller[1], Carlo Ciaccia[1], Artem Kononov[1], Erik P. A. M. Bakkers[2], Joost Ridderbos[3], Andreas Baumgarner[1,4], and •Christian Schönenberger[1,4] — [1]Dep. Physics, Univ. of Basel, Basel, Switzerland — [2]Dep. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, The Netherlands — [3]MESA+ Inst. of Nanotechnology, Univ. of Twente, Enschede, The Netherlands — [4]Swiss Nanoscience Institute, Univ. of Basel, Basel, Switzerland

Transmon qubits are currently the most popular solid-state platform for small and intermediate scale quantum technology applications. However, there are several challenges, such as the large size and hence the difficulty in scaling to many qubits, the sensitivity to flux noise and the associated power load for driving qubits through flux lines.

A possible solution are semiconductor-superconductor hybrid systems called gatemon qubits where the Josephson junction is realized by a gate-tunable weak link. Such gatemons have intensively been studied in III-V semiconductor 2D and 1D platforms. But only recently work

has been started on using type-IV semiconductors to realize gatemons. Here, we present a gatemon qubit based on a Ge/Si core-shell nanowire Josephson junction. On this new platform we demonstrate the electrical tunability and coherent manipulation, with coherence times on par with other gatemon platforms. We also demonstrate that these junctions are highly transmissive opening a way to realize parity protected 4e gatemon devices.

HL 11.3 Mon 15:30 EW 203

**Real-Time Processing of Quantum Measurements: Quantum Polyspectra Approach to the Weak, Strong, and Single Photon Regime** — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, Germany

Quantum polyspectra have recently been successfully utilized in the evaluation of continuous quantum measurement records across weak, strong, and single photon regimes. This analysis is conducted by comparing experimental quantum polyspectra with their theoretical counterparts [1]. Our freely accessible Python library, SignalSnap [2], offers an efficient GPU-based method for calculating the polyspectra. Expanding on this groundwork, we introduce new software for the real-time evaluation of quantum measurement data with MHz bandwidth using polyspectra. This approach enables immediate processing and interpretation of quantum measurements. The goal is to achieve real-time characterization of quantum systems by estimating their Liouvillians. This capability is crucial for deepening our understanding of quantum dynamics. Real-time evaluation of measurements allows experimentalist to find interesting parameter settings already in the lab or to identify obvious errors in the experiment, like drift, missalignment, or unwanted external noise.

[1] Sifft et al., Phys. Rev. Research 3, 033123 (2021).
[2] https://github.com/MarkusSifft/SignalSnap

HL 11.4 Mon 15:45 EW 203

**Multiband $k \cdot p$ theory for hexagonal germanium** — •Yetkin Pulcu[1], Janos Koltai[2], Andor Kormanyos[3], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Biological Physics, Eötvös Loránd University, Budapest, Hungary — [3]Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary

The direct bandgap found in hexagonal germanium and some of its alloys with silicon allows for an optically active material within the group-IV semiconductor family with various potential technological applications. However, there remain some unanswered questions regarding several aspects of the band structure, including the strength of the electric dipole transitions at the center of the BZ. In this work [2], using 10 band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian with SOC near the $\Gamma$ point, we obtain a self-consistent model that describes 2H-Ge via fitting to *ab initio* data. To understand the weak dipole coupling between the lowest conduction band and the top valance band, we start from a spinless 12-band model and show that when adding spin-orbit coupling, the lowest conduction band hybridizes with a higher-lying conduction band. Additionally, we derive the effective low-energy Hamiltonian for the conduction bands for the possible spin dynamics and nanostructure studies. Finally, we include the effects of a magnetic field and predict the electron and hole g-factor of the conduction and valence bands.

[1] Pulcu, Yetkin, et al. "Multiband $k \cdot p$ theory for hexagonal germanium." arXiv preprint arXiv:2310.17366 (2023).

HL 11.5 Mon 16:00 EW 203

**Spin-orbit coupling of color centers for quantum applications** — •Mirjam Neubauer, Maximilian Schober, Witold Dobersberger, and Michel Bockstedte — Institute for Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

Color centers in semiconductors, such as the NV-center in diamond, the silicon vacancy ($V_{Si}^-$), and the di-vacancy ($V_C V_{Si}$) in 4H-silicon carbide (4H-SiC), are potential candidates for quantum bits (qubits). Manipulating the spin optically involves exciting the fundamental high-spin multiplet and intersystem crossing (ISC), which includes spin-orbit, spin-spin, and spin-phonon couplings. These interactions, together with the zero-field splitting of ground and excited states, enable diverse spin-photon protocols. To optimize the engineering of such interfaces, a comprehensive understanding of spin-selective interactions and resulting spin-relaxation pathways is crucial. Recent experiments regarding the $V_{Si}^-$ in SiC have revealed spin-dependent lifetimes and intercrossing rates using an effective model that considers only one or two out of the five predicted intermediate states [1]. Here we address this issue. We employ our extended CI-cRPA approach for correlated defect states [2] to calculate the spin-orbit and spin-spin coupling. We present a fine structure of the quartet states of $V_{Si}^-$ consistent with existing literature. Based on our calculations, we discuss the ISC and spin-relaxation paths.

[1] N. Morioka et al.Phys. Rev. Appl. **17** 054005 (2022).
[2] M. Bockstedte, et al., npj Quant Mater **3**, 31 (2018).

HL 11.6 Mon 16:15 EW 203

**Protocols to measure the non-Abelian Berry phase by pumping a spin qubit through a quantum-dot loop** — •Baksa Kolok[1] and Andras Palyi[1,2] — [1]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]MTA-BME Quantum Dynamics and Correlations Research Group, Muegyetem rkp. 3., H-1111 Budapest, Hungary

A quantum system constrained to a degenerate energy eigenspace can undergo a nontrival time evolution upon adiabatic driving, described by a non-Abelian Berry phase. This type of dynamics may provide logical gates in quantum computing that are robust against timing errors. A strong candidate to realize such holonomic quantum gates is an electron or hole spin qubit trapped in a spin-orbit-coupled semiconductor, whose twofold Kramers degeneracy is protected by time-reversal symmetry. Here, we propose and quantitatively analyze protocols to measure the non-Abelian Berry phase by pumping a spin qubit through a loop of quantum dots. One of these protocols allows to characterize the local internal Zeeman field directions in the dots of the loop. We expect a nearterm realisation of these protocols, as all key elements have been already demonstrated in spin-qubit experiments. These experiments would be important to assess the potential of holonomic quantum gates for spin-based quantum information processing.

**15 min. break**

**Invited Talk** HL 11.7 Mon 16:45 EW 203

**Strategic wafer-scale creation of telecom single-photon emitters in silicon for large-scale quantum photonic integrated circuits** — •Yonder Berencen — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328, Dresden, Germany

Indistinguishable single-photon sources at telecom wavelengths are crucial for transmitting quantum information over long distances with minimal losses, facilitating secure quantum communication and a modular approach to quantum computing. Monolithic integration of these sources with reconfigurable photonic elements and single-photon detectors in a silicon chip is vital for scalable quantum hardware, such as quantum photonic integrated circuits (QPICs). While many necessary components for QPICs are available, the lack of on-chip single-photon emitters in silicon has hindered practical implementation on the nanoscale. This study presents two wafer-scale protocols, demonstrating quasi-deterministic creation of single G and W telecom-wavelength color centers in silicon with over 50% probability. Both protocols are compatible with current silicon technology, enabling fabrication of single telecom quantum emitters at desired nanoscale positions on a silicon chip. These results offer a clear pathway for industrial-scale photonic quantum processors with technology nodes below 100 nm, overcoming a critical obstacle in the development of scalable quantum photonic hardware.

HL 11.8 Mon 17:15 EW 203

**Color centers in hexagonal boron nitride for quantum memories.** — •Chanaprom Cholsuk[1], Asli Cakan[2], Sujin Suwanna[3], and Tobias Vogl[1,2] — [1]Abbe Center of Photonics, Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany — [2]Department of Computer Engineering, School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [3]Optical and Quantum Physics Laboratory, Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

A quantum memory is essential for large-scale quantum networks. While several quantum memories have been developed so far, many cases remain unable to meet all requirements entirely i.e. long storage time, selective compatibility, and high memory efficiency. This work therefore proposes a quantum memory from color centers in hexagonal

boron nitride in a cavity based on the Raman scheme with Lambda-type (Λ) energy levels. 257 triplet and 211 singlet spin electronic transitions have been characterized by density functional theory and classified with quantum applications. The result suggests that some defects inherit the Λ electronic structures under neutral charge, whereas some require charge-state manipulation. Further, the required quality factor and bandwidth provide a reasonable range for achieving a 95% writing efficiency. Consequently, this work contributes to realizing hBN as a quantum memory for future quantum networks.

HL 11.9 Mon 17:30 EW 203

**Coherence properties of exciton-polariton condensates in a long lifetime microcavity** — •Yannik Brune[1], Elena Rozas[1], Kirk Baldwin[2], Loren Pfeiffer[2], David Snoke[3], and Marc Assmann[1] — [1]Department of Physics, Technische Universität Dortmund, Dortmund 44227, Germany — [2]Department of Electrical Engineering, Princeton University, New Jersey 08544, USA — [3]Department of Physics & Astronomy, University of Pittsburgh, Pittsburgh 15260, USA

The coherence properties of all-optically excited polariton condensates are typically hindered by the interactions with the concurrently excited incoherent background. We circumvent this restriction by using an annular shaped CW excitation beam, acting as a trapping potential in combination with long lifetime polaritons in a high Q-factor microcavity. Our approach enables the separation of the condensation area from the excitation area. The condensate properties are then examined using two-channel homodyne detection. This allows us not only to determine $g^2(0)$ but also access its Husimi-Q distribution and further properties like quantum coherence. These results provide a deeper understanding of the polariton condensate behavior beyond the condensation threshold. Our findings offer new insights into the use of CW pumped polariton condensates as ultralow threshold coherent light source.

HL 11.10 Mon 17:45 EW 203

**Theory of valley physics in SiGe quantum dots** — •Jonas de Lima and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

The weak spin-orbit coupling and the nuclear zero-spin isotopes of silicon and germanium make Si/Ge quantum dots an ideal host for semiconductor spin qubits. However, the degeneracy of the conduction band minima of bulk silicon, known as valleys, limits the performance and scalability of quantum information processing, because the valley degree of freedom competes with the spin as a low-energy two-level system. The valley degeneracy is lifted in quantum dots in Si/SiGe heterostructures due to biaxial strain and a sharp interface potential, but the reported valley splittings are often uncontrolled and can be as low as 10 to 100 $\mu$eV. This presentation will discuss in detail the main challenges for the enhancement and control of the valley splitting in silicon quantum dots. In addition, it will describe a new three-dimensional model within the effective mass theory for the calculation of the valley splitting in Si/SiGe heterostructures, which takes into account concentration fluctuations at the interface and the lateral confinement. With this model, we predicted the valley splitting as a function of various parameters, such as, the width of the interface, the electric field and the size and location of the quantum dot.

## HL 12: Semiconductor Lasers I

Time: Monday 15:00–16:45 Location: EW 561

HL 12.1 Mon 15:00 EW 561

**Multi-Hole-Aperture VCSELs to remove the saturation current barrier** — •Sicong Tian[1,2], Mansoor Ahamed[1,3], Georgiy Sapunov[1], and Dieter Bimberg[1,2] — [1]imberg Chinese-German Center for Green Photonics, Changchun Institute of Optics, Fine Mechanics, and Physics, Chinese Academy of Sciences, Changchun 130033, PR China — [2]Center of Nanophotonics, Institute of Solid State Physics, Technische Universität Berlin, Berlin D-10632, Federal Republic of Germany — [3]The University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

Novel design of Vertical-Cavity Surface-Emitting Lasers is presented leading to a strong reduction of thermally induced band gap shift as a function of current. The aperture is realized through dry etching geometrically variable arrangements of deep holes and subsequent oxidation. The blind holes are then filled with gold resulting in an effective heat drain technology. The shape and size of the aperture depend on the arrangement of holes [1]. Larger output power, rollover current, single-mode emission, and reduced series resistance are demonstrated. In addition, pseudo-single-mode multi-aperture VCSELs are enabled [2]. Refferences [1] G. Larisch, S.C. Tian, and D. Bimberg, Radiation Emitter, EP2020192355. [2] G. Larisch, S.C. Tian, and D. Bimberg, Radiation Emitter, EP2021168265.

HL 12.2 Mon 15:15 EW 561

**Tuning nanowire lasers via hybridization with tailored dye molecules** — •Edwin Eobaldt, Leon Kross, Jakob Wurschi, Aurelia Eberhard, Marco Grünewald, Daniel Costabel, Kalina Peneva, and Carsten Ronning — Friedrich-Schiller-Universität, Jena, Deutschland

Among the myriad nanomaterials, semiconductor nanowires have garnered considerable scientific attention as promising candidates for realizing nano-scaled coherent light sources and all-optical circuits. This interest stems from their notable waveguiding properties and intrinsic ability to lase under high excitation. Nevertheless, achieving a precise control over their lasing properties, such as emission wavelength and lasing threshold, is crucial for a diverse range of applications. In this context, the hybridization of nanowires with tailored molecules emerges as a potential avenue, offering new control mechanisms through efficient charge and energy transfer processes at the heterointerface. To illustrate this concept, we chose to hybridize ZnO nanowires with perylene-based dye molecules, leveraging their exceptional chemical and optical stability. Notably, these molecules provide the advantage of easily tuning their optical gap across a broad spectral range through chemical functionalization. This study employs comparative micro-photoluminescence measurements to explore the impact of these molecules on the nanowire lasing properties. Specifically, we demonstrate how different chemical functionalizations and varying amounts of dyes enable nanowire wavelength tuning.

HL 12.3 Mon 15:30 EW 561

**Growth, fabrication, and characterization of site-controlled quantum dots microcavity arrays based on buried-stressor approach** — •Kartik Gaur, Sam Baraz, Lukas Dworaczek, Sarthak Tripathi, Imad Limame, Ching-Wen Shih, Martin Podhorsky, Aris Koulas-Simos, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

The buried-stressor approach 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 the growth, fabrication, and characterizations of SCQD microcavity arrays consisting of spectrally homogeneous single photon sources. Various optimizations in the growth process are explored through simulations, with subsequent samples grown using metal-organic chemical vapor deposition (MOCVD) to achieve position, number, and emission energy-controlled QDs. 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 ($\mu$PL) spectroscopy. Furthermore, quantum optical characterizations such as second-order autocorrelation, visibility measurements, etc. are also performed on these SCQD arrays. The comprehensive understanding of the intricacies involved in the growth and characterization of SCQDs offers a roadmap for advancing quantum information technology.

HL 12.4 Mon 15:45 EW 561

**Investigation of different QW arrangements in the deep red laser emission range for VECSELs in a V-shaped resonator** — •Rebecca Rühle, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In this work we investigate the influence of the quantum well (QW) distribution of a VECSEL (Vertical external-cavity surface emitting laser) on its optical output power. One parameter is the layer thickness, since a thicker laser structure is associated with higher temperatures in the active region. In order to vary the thickness, three different QW distributions are examined. The VECSEL chip consists of a Al(0.3)GaAs/Al(0.95)GaAs DBR and an active region with InGaAsP QWs, grown with a MOVPE (metal-organic vapor-phase epitaxy). For the investigated VECSELs, the total number of QWs is kept approximately at the same to optain a better comparability. The exact structure of the investigated VECSELs consists of 11x1, 6x2 and 4x3 InGaAsP QWs embedded in a GaInP barrier for laser emission at 770nm. Power measurements were used to investigate and analyze the performance of the v-shaped resonator and VECSEL structures.

HL 12.5 Mon 16:00 EW 561

**265 nm AlGaN based laser heterostructures using distributed polarization doping** — •Lennard Zinsilowski[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Giulia Cardinali[1], Luca Sulmoni[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

In this study the growth of 265 nm laser diode heterostructures by metalorganic vapor phase epitaxy (MOVPE) implementing distributed polarization doping is investigated. P-type AlGaN layers using distributed polarization doping (DPD) have been recently developed to achieve higher conductivity than p-doped AlGaN:Mg layers, which exhibit increasing resistivities due to increasing ionization energies with higher Al mole fractions. Through a pseudomorphically grown grading of the $Al_xGa_{1-x}N$ layers polarization charges are generated in the layer, inducing free hole carriers even in the absence of Mg dopants. The impact of the active zone growth conditions, structural design and also the DPD design regarding the electrical properties of the laser diodes were studied aiming to achieve high current injection efficiencies. Pulsed on-wafer measurements of 5 $\mu$m x 800 $\mu$m large devices at a current of 1 A (25 kA/cm$^2$) show voltages around 30 V and a series resistance of 10 Ω. The DPDs show a high durability sustaining current densities of more than 100 kA/cm$^2$ for different geometries. This shows a promising approach towards UV-C laser diodes working on sapphire.

HL 12.6 Mon 16:15 EW 561

**Polarized-resolved Raman scattering of epitaxially grown (Si)GeSn layers** — •Agnieszka Corley-Wiciak[1], Shunda Chen[2], Omar Concepción[3], Marvin H. Zoellner[1], Detlev Grützmacher[3], Dan Buca[3], Tianshu Li[2], Giovanni Capellini[1,4], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]Department of Civil and Environmental Engineering, George Washington University, Washington USA — [3]Peter Grünberg Institute 9 (PGI-9) and JARA-Fundamentals of Future Information Technologies, Juelich, Germany — [4]Dipartimento di Scienze, Università Roma Tre, Roma,

Silicon-Germanium-tin (SiGeSn) alloys are gaining popularity due to their potential applications in photonics, optoelectronics, microelectronics, and thermoelectrics. To accomplish this, it is critical to accurately assess the effect of composition, strain, and deposition method on the crystal quality. Raman spectroscopy as an experimental tool for probing vibrational modes allows a detailed study of these qualitites. Here we investigate the role of Sn incorporation on the vibrational properties of (Si)GeSn epitaxial layers using polarized Raman spectroscopy and numerical simulations. The nature of the disordered-assisted spectral feature can be ascertained through a comparative analysis. It comprises two modes: one associated with the vibration of Ge atoms that Sn neighbors do not impact, and the disorder activating specific mode. This provides a framework for understanding the vibrational properties in SiGeSn alloys, particularly concerning the impact of the local ordering of different atomic species.

HL 12.7 Mon 16:30 EW 561

**Free space emission spectra and bandwidths of vertical cavity surface emitting lasers** — •Pouria Emtenani[1], Nasibeh Haghighi[1], Martin Zorn[3], Markus R Wagner[1,2], and James A Lott[1] — [1]Technical University of Berlin — [2]Paul-Drude-Institut Berlin — [3]JENOPTIK Optical Systems GmbH, Berlin

We measure and analyze the free space (across air) emission spectra and small-signal modulation bandwidths of top-emitting 980 nm vertical cavity surface emitting lasers (VCSELs) and electrically parallel VCSEL arrays. We design and fabricate the VCSELs at the Technical University of Berlin [1] and test them using on-wafer high-frequency probing. The VCSEL emission is collected into a standard OM2 multiple-mode optical fiber patch cord with a length of 10 meters which in turn directs the optical signal into a triplet-lens fiber collimator. The light exits the fiber collimator as a free space beam. A second triplet-lens fiber collimator collects the light and directs it into a second OM2 fiber patch cord with a length of 3 meters which then directs the optical signal into an optical spectrum analyzer or onto a high bandwidth photodiode connected to a 2-port vector network analyzer. We achieve a free space bandwidth across 0.4 and 4.5 meters of air of 16 GHz for a 19-element array and 25 GHz for a single VCSEL, a crucial first step toward free space data transmission at 25 Gbps or faster for future, sixth generation optical wireless communication systems, Internet of Things connectivity, and next generation light fidelity systems. [1] N. Haghighi, Dissertation. [online] https://depositonce.tu-berlin.de/handle/11303/16321

## HL 13: Poster I

Topics:
- Heterostructures, interfaces and surfaces
- Optical properties of semiconductors
- Organic semiconductors
- Oxide semiconductors
- Perovskites and photovoltaics
- Spin phenomena in semiconductors
- THz and MIR physics in semiconductors

Time: Monday 15:00–18:00 Location: Poster E

HL 13.1 Mon 15:00 Poster E

**"A Comparative Analysis of Two Different Full-Wafer Photoluminescence Spectroscopy Mappers"** — •Elias Kersting, Alexander Schauerte, Hans-Georg Babin, Andreas Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

Photoluminescence spectroscopy (PL) is an indispensable method for investigating the optical properties of semiconductor heterostructures. Spectroscopy of a complete wafer is necessary to obtain important growth parameters of samples grown with a molecular beam epitaxy (MBE) system. We present two different approaches for the construction of a fully automated 3-inch PL spectroscopy Mapper. The first setup uses mirrors as optical components and a movable cryostat. In the second setup, the heavy cryostat is fixed and a movable, lightweight optical system of lenses is used instead. The advantages and disadvantages are discussed and measurements on local droplet etched GaAs quantum dots are compared.

HL 13.2 Mon 15:00 Poster E

**Quantifying quantum coherence in multi-mode polariton condensates** — •Maximilian Nürmberger, Franziska Barkhausen, Xuekai Ma, Jan Sperling, and Stefan Schumacher — Department of Physics, CeOPP, and PhoQS, Paderborn University, Germany

One of the main challenges when engineering future quantum devices based on light-matter interaction is achieving resourceful and long-term coherent quantum states. We theoretically investigate quantum features of a polariton system and quantify the amount of quantum coherence that results from the quantum superposition of Fock states, constituting a measure of the resourcefulness for modern quantum protocols. We use phase-space quasi probability distributions of macroscopic polariton states to quantify changes in the quantum coherence beyond the condensation threshold [1,3] and calculate the time evolution using a regularized Glauber-Sudarshan representation [2,3]. Furthermore, we include the polarization degree of freedom and expand our calculations into orbital angular momentum (OAM) space to investigate the quantum coherence of multi-mode systems. In doing so we can calculate the quantum coherence of different vortex states in polariton condensates. We theoretically study vortices excited non-resonantly in an optically induced ring-shaped potential. By introducing a resonant control pulse in either polarization component, we can switch between different vortex-states [4]. [1] C. Lüders et al., PRX Quantum 2, 030320 (2021). [2] C. Lüders et al., Phys. Rev. Lett. 130, 113601 (2023). [3] C. Lüders et al., Opt. Mater. Express 13, 2997-3035 (2023). [4] M. Pukrop et al., Phys. Rev. B 101, 205301 (2020).

HL 13.3 Mon 15:00 Poster E

**Two-photon excitation channels in CuI** — •Andreas Müller[1], Leonard Käferstein[1], Lukas Trefflich[1], Steffen Blaurock[2], Harald Krautscheid[2], Marius Grundmann[1], and Chris Sturm[1] — [1]Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, 04103 Leipzig, Germany

Having recently identified strong two-photon absorption (2PA) in CuI [1], we're examining the excitation channels linked to this phenomenon.

We investigate the interferometric autocorrelation (IAC) function of CuI across various excitation energies to discern distinct excitation channels in 2PA-induced photoluminescence (PL). Probing near the 2PA edge (795 nm), the broadening of the IAC function of CuI is similar to the pulse duration of the laser (FWHM ≈ 200 fs) suggesting an excitation assisted by a virtual level. In contrast, probing with 460 nm, a different IAC shape emerges with significant broadening (FWHM ≈ 475 fs). Given the predicted presence of a defect level at this energy [2] and the alignment with the extension of the DAP band in this excitation range, we attribute these alterations to 2PA process assisted by a real level. Similar variations in the IAC function have been documented in prior literature on GaAs [3], which supports our interpretation. We estimate a real-level lifetime of approximately 220 fs.

[1] A. Müller *et al.*, Appl. Phys. Lett. **123**, 122103 (2023)
[2] S. Koyasu *et al.*, J. Appl. Phys **125**, 115101 (2019)
[3] T. Hattori *et al.*, Jpn. J. Appl. Phys. **39**, 4793 (2000)

HL 13.4 Mon 15:00 Poster E

**On-chip lateral Si:Te PIN photodiodes for room-temperature detection in the telecom optical wavelength bands** — Mohd Saif Shaikh[1,2], Shuyu Wen[1,3], Mircea-Traian Catuneanu[2], Mao Wang[4], Artur Erbe[1,2], Slawomir Prucnal[1], Lars Rebohle[1], •Shengqiang Zhou[1], Kambiz Jamshidi[2], Manfred Helm[1,2], and Yonder Berencén[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Dresden University of Technology, 01062 Dresden, Germany — [3]Institute of Semiconductors, Chinese Academy of Sciences, Bejing, China — [4]Sichuan Normal University, Chengdu 610101, China

Photonic integrated circuits require photodetectors that operate at room temperature with sensitivity at telecom wavelengths and are suitable for integration with planar complementary-metal-oxide-semiconductor (CMOS) technology. Silicon hyperdoped with deep-level impurities is a promising material for silicon infrared detectors because of its strong room-temperature photoresponse in the short-wavelength infrared region caused by the creation of an impurity band within the silicon band gap. In this work, we present the first experimental demonstration of lateral Te-hyperdoped Si PIN photodetectors operating at room temperature in the optical telecom bands. We provide a detailed description of the fabrication process, working principle, and performance of the photodiodes, including their key figure of merits. Our results are promising for the integration of active and passive photonic elements on a single Si chip, leveraging the advantages of planar CMOS technology.

HL 13.5 Mon 15:00 Poster E

**High-reflectivity $Al_2O_3/Al_{0.3}Ga_{0.7}As$ distributed Bragg reflectors and microcavities for photon Bose-Einstein-condensates in GaAs quantum wells** — •Lara Schmieder[1,3], Nils von den Driesch[2,3], Yurii Kutovyi[1,3], Siqi Qiao[1,3], Christoph Krause[2], Benjamin Bennemann[2], and Alexander Pawlis[1,2,3] — [1]PGI-9, Forschungszentrum Jülich GmbH — [2]PGI-10, Forschungszentrum Jülich GmbH — [3]JARA-FIT, Jülich Aachen Research Alliance

Significant present research is focused on the realization of Photon-Bose-Einstein-Condensates (P-BECs) for applications in quantum technology. We propose a scalable chip-architectur composed of III-V semiconductor microcavities with GaAs quantum wells. The latter are directly grown between high-reflectivity AlOx based Distributed Bragg Reflectors (DBRs) to form a high-finesse microcavity. In order to reach the thermalization conditions of a semiconductor based P-BEC, extremely high reflectivity of the DBRs is required.

We meet these condition by establishing AlOx based DBRs fabricated via a combined nanostructuring and wet-oxidation process of as-grown $AlAs/Al_{0.3}Ga_{0.7}As$ superlattices. Reflectivity measurements of our AlOx based Bragg reflectors owe much higher reflectivity as standard $AlAs/Al_{0.3}Ga_{0.7}As$ Bragg-mirrors with similar number of periods. Quantitative analysis of microcavities with AlOx based DBRs confirm that 8-fold stacks are already sufficient to achieve high enough finesse to overcome the above mentioned thermalization limit.

HL 13.6 Mon 15:00 Poster E

**Manipulating spectral topology and exceptional points by nonlinearity in non-Hermitian polariton systems** — Jan Wingenbach, Stefan Schumacher, and •Xuekai Ma — Physics Department and CeOPP, and PhoQS, Paderborn University, Germany

Exceptional points (EPs) are singularities in parameter space at which two or more eigenstates coalesce. Such singularities occur exclusively in non-Hermitian systems which are subject to gain and loss and exhibit non-orthogonal eigenvectors and complex eigenvalues. Due to their intriguing spectral topology EPs have attracted considerable attention in a broad range of physical systems, with potential sensing applications driving much of the present research in this field [1]. We investigate the EPs in systems with significant nonlinearity, exemplified by a nonequilibrium exciton-polariton condensate. Polaritons are quasiparticles, formed due to the strong coupling of photons and excitons in planar semiconductor microcavities. With the possibility to control loss and gain and nonlinearity by optical means, this system allows for a comprehensive analysis of the interplay of nonlinearities (Kerr-type and saturable gain) and non-Hermiticity [2]. Not only do we find that EPs can be intentionally shifted in parameter space by the saturable gain, we also observe intriguing rotations and intersections of Riemann surfaces and find nonlinearity-enhanced sensing capabilities. These results illustrate the potential of tailoring spectral topology and related phenomena in non-Hermitian systems by nonlinearity. [1] J. Wiersig, et al., Photonics Research 8, 9 (2020). [2] J. Wingenbach, et al., arXiv:2305.04855 (2023).

HL 13.7 Mon 15:00 Poster E

**Cathodoluminescence study of point and structural defects in bottom-up GaN nanowires** — •Mikel Gómez Ruiz[1], Matt Brubaker[2], Kris Bertness[2], Manfred Ramsteiner[1], Oliver Brandt[1], and Jonas Lähnemann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Germany — [2]National Institute of Standards and Technology, USA

Luminescence techniques are inherently sensitive to the presence of both radiative and nonradiative defects. In this work, we investigate the prevalence and distribution of both point and structural defects in GaN nanowires (NWs) by low-temperature (10 K) cathodoluminescence (CL) hyperspectral line scans along the NW axis. Ordered arrays of NWs are grown by selective-area molecular beam epitaxy using a $Si_3N_4$ mask on a N-polar GaN template on Si. The CL intensity of single NWs is observed to vary along the NW axis. During initial NW growth, impinging Ga atoms can react with the $Si_3N_4$ mask leading to the unintentional incorporation of Si into the NW. The incorporation is gradually reduced once the NW height is approximately equal to their distance, where shadowing prevents the direct impingement of Ga atoms on the mask. The Fermi-level pinning at the NW side facets results in internal electric fields, whose spatial extent depends on the Si concentration and the NW diameter. These fields can dissociate excitons as well as shallow donors and acceptors, thus reducing the corresponding radiative emission intensity. A gradient in Si doping can thus explain the change in emission intensity. This Si doping also

causes most of the NWs to have inversion domain boundaries.

HL 13.8 Mon 15:00 Poster E

**Topological edge and corner states in coupled wave lattices in nonlinear polariton condensates** — •Tobias Schneider[1], Wenlong Gao[2], Thomas Zentgraf[1,3], Stefan Schumacher[1,3,4], and Xuekai Ma[1] — [1]Physics dept. CeOPP, Paderborn University, Germany — [2]EIT Institute for Advanced Study, Ningbo, China — [3]Physics dept. PhoQS, Paderborn University, Germany — [4]Wyant College of Optical Sciences, University of Arizona, Tucson, USA

Topological states are of great interest due to their robustness against perturbations, hence they have been widely investigated in many physical systems including microcavity exciton polaritons[1]. In this work, we explore topological states in exciton polariton condensates in our newly designed double-wave (DW) lattices[2]. Exciton polaritons are quasiparticles composed of excitons and photons in semiconductor microcavities and show strong repulsive nonlinearity. The 1D DW chains we proposed enable multiple types of edge states in both the linear and the nonlinear regime, in which they are shown to be multistable. The strong nonlinearity of polaritons can also lead to the formation of new types of edge states that originate from the bulk eigenstates, i.e. nonlinearity-enhanced edge localization. The 1D lattice can be expanded into a 2D lattice structure, with SSH like structures in the new dimension. The combination of the perpendicularly DW and SSH lattices allows for the formation of additional higher-order topological insulator states (0D corner states). These corner states are also shown to be multistable in the nonlinear regime.[1] S. Klembt et al., Nature 562, 552 (2018).[2] T. Schneider et al., arXiv:2303.12593 (2023).

HL 13.9 Mon 15:00 Poster E

**Bulk-Material Supercontinuum Generation for Temporal Compression of Ultrafast Laser Pulses** — •Olga Resel, Hana Hampel, Daniel Hipp, Adrian Kirchner, and Martin Schultze — Institute of Experimental Physics, Graz University of Technology, Austria

For the generation of ultrashort laser pulses spectral broadening of the output of commercially available short-pulse laser sources is essential. This can be achieved by nonlinear light - matter interaction. Here we studied self-phase modulation of a commercial Yb:KGW laser system (PHAROS from Light Conversion) in fused silica. In a first step, the spectrum and the interferometric autocorrelation of the unfocused laser beam, propagating through fused silica, were measured and analysed in contrast to measurements without fused silica in the beam path. The obtained spectra were compared to numerical simulations of self-phase modulation with the experimental laser parameters as well as the Fourier transform of the initial spectrum as input. Although dispersion was neglected in the computations, the results and the experimental observations are in excellent agreement. In a second step, limits of self-phase modulation were explored by increasing beam intensities using a focused laser beam. The spectra and further the interferometric autocorrelations of the broadened pulses were measured. At the limit of self-phase modulation, even a white light supercontinuum was observed. Based on these measurements, it could be possible to achieve a 50% reduction of the pulse duration, if proper dispersion compensation can be implemented.

HL 13.10 Mon 15:00 Poster E

**Energy-Momentum-Resolved Spectroscopy of Chiral Hybrid Perovskites** — •Caroline Aschendorf[1], Jonathan Zerhoch[1,2,3], Shangpu Liu[1,2,3], and Felix Deschler[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Walter Schottky Institut, Technische Universität München — [3]Physics Department, TUM School of Natural Sciences, Technische Universität München

Energy-momentum-resolved spectroscopy allows for highly sensitive photoluminescence measurements, revealing the orientation of the emission dipole moment. Different momentum intensity profiles distinguish between in-plane (IP) and out-of-plane (OP) exciton orientations through s- and p-polarized components of the emitted light. Of particular interest is the investigation of the novel chiral 2D hybrid metal-halide perovskite (HMHP) $(R/S)$-3BrMBA$_2$PbI$_4$, which exhibits a high photoluminescence quantum yield (PLQY) of up to 39% and circularly polarized photoluminescence (CPL) of up to 52%. Energy-momentum spectra were acquired for thin films and facets of single crystals of $(R/S)$-3BrMBA$_2$PbI$_4$, $(R/S)$-4BrMBA$_2$PbI$_4$, BA$_2$PbI$_4$, and the inorganic 3D perovskite CsPbBr$_3$. This allowed the modeling of the in-plane (IP) to out-of-plane (OP) exciton ratio, revealing a notable distribution towards OP excitons in certain materials.
The study of CPL in chiral materials aims to investigate the impact of chirality on exciton orientation. This knowledge is crucial for advancing chiral HMHP development with higher CPL and PLQY, holding promise for chiroptical applications and chiral spintronics.

HL 13.11 Mon 15:00 Poster E

**Multidimensional Coherent Spectroscopy on naturally grown $Cu_2O$** — •Mariam Harati, Julian Heckötter, Binodbihari Panda, Simon Siegeroth, and Marc-Alexander Assmann — Technische Universität Dortmund, Dortmund, Deutschland

Excitons are elementary excitations in various electronic systems. They play a fundamental role in solid state quantum technology and thus building new optoelectronic devices. Especially the optical prosperities of excitons in Cuprous Oxide ($Cu_2O$) are of significant interest in the field of precision sensor technologies since Rydberg-Excitons with large quantum numbers $n$ can be created in this material (T. Kazimierczuk et al. Nature 514, 343 (2014)). In this work, we present Multidimensional Coherent Spectroscopy (MDCS) of Rydberg-Excitons of the yellow series in naturally grown $Cu_2O$. It allows us to measure the third order nonlinear optical response of $Cu_2O$ and to characterize inhomogeneity and coupling. In order to perform MDCS a collinear spectrometer is used. In addition to the spectrometer, the sample is scanned along the plane perpendicular to the optical axis. This provides us with hyperspectral images of impurities and excitons.

HL 13.12 Mon 15:00 Poster E

**In situ time-resolved photoluminescence measurement in the PEC environment** — •Peter Kleinschmidt, Elias Hartung, Lucas Krätschmer, David Ostheimer, and Thomas Hannappel — TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials, 98693 Ilmenau

Recombination properties of minority charge carriers are crucial for the optoelectronic performance of a many semiconductor devices. Time-resolved photoluminescence (TRPL) measurement, based on time-correlated single photon counting, provides direct access to the effective minority charge carrier lifetime. Typically, this is carried out separately from preparation and operation of devices. We have developed a flexible TRPL-setup with a remote measuring head which allows measurement in different environments. We demonstrate measurement of charge carrier lifetimes in a photo-electrochemical cell, providing access to device performance and degradation in this environment. The measurement can be performed in correlation with photo-electrochemical operation of the sample and enables observation of different influences on the optoelectronic device properties.

HL 13.13 Mon 15:00 Poster E

**Optimization of vertically graded $Mg_xZn_{1-x}O$ layers for the use in wavemeters** — •Christoph Brunhuber, Lukas Trefflich, Daniel Splith, Chris Sturm, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany

To determine the wavelength of monochromatic radiation, a new design for a wavemeter was proposed, that is forward-looking, monolithic and ultra-compact [1]. It consists of two vertically stacked, photosensitive layers, separated by a transparent, insulating layer. The top layer has a vertically graded alloy composition in order to achieve spectral sensitivity. The ratio of the photocurrents generated in the two absorber layers relates to the wavelength of the incident radiation.

We realized such wavemeter devices using a $Mg_xZn_{1-x}O$ alloy system. Within the graded absorber layer the Mg-content increases from $x = 0$ to $x \approx 0.4$. The two absorber layers were deposited on opposite sides of a sapphire substrate by pulsed laser deposition, using a vertical continuous composition spread (VCCS-PLD) technique to obtain the graded layer. Here, we discuss the optimization of the vertically graded $Mg_xZn_{1-x}O$ layer. For structural analysis XRD $2\theta$–$\omega$-scans were performed. The functionality of the wavemeters was confirmed by spectrally resolved photocurrent measurements under illumination with monochromatic light. The photocurrent-ratio shows a wavelength dependency similar to the theoretically calculated one [1].

[1] M. Grundmann. Phys. Stat. Sol. A **215**, 1800651 (2018)

HL 13.14 Mon 15:00 Poster E

**Resonant Raman scattering at split-off band exciton in CuI** — •R. Hildebrandt[1], S. Blaurock[2], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, Germany — [2]Universität Leipzig,

Institute of Inorganic Chemistry, Germany

We investigate the resonant Raman spectrum of copper iodide (CuI), and observed up to ten consecutive LO-phonon scattering processes for the split-off band exciton. This exciton is energetically isolated and located above the fundamental bandgap. The resonance condition is varied by using excitation wavelengths of 355 nm, 325 nm and 320 nm, which are located above and below the respective exciton energy of 335nm.

This resonant interaction of excitons and phonons is mediated via the Fröhlich interaction and can give access to fundamental material characteristics such as effective masses, electron-phonon coupling and their wave-vector dependence. Dipole-forbidden transitions can be investigated or localized modes can be used for precise determination of doping concentrations [1]. The observed multiple LO-phonon scattering processes are typical for polar semiconductors[2] and contain information for exciton damping constants, relaxation times as well as acoustic phonon dispersion characteristics [3]. The therewith-derived properties of CuI will be discussed in this work.

[1] Y. Zhang, J. Semicond., **40**, 091102, 2019.
[2] R. Leite, J., Phys. Lett., **22**, 780, 1969.
[3] P. Yu and M. Cardona, Fundamentals of Semiconductors, 2010.

HL 13.15 Mon 15:00 Poster E

**Electro-optical phase change devices based on nanocrystalline graphite heaters for integrated photonic circuits** — •Niklas Vollmar[1], Anna Ovvyan[2], Wolfram Pernice[2], and Martin Salinga[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Kirchhoff-Institute for Physics, University of Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

In-memory computing with integrated photonic circuits is promising due to high bandwidth and low latency. In such systems, phase change materials (PCMs) can be used as compact and non-volatile modulators: the pronounced contrast in permittivity between their crystalline and amorphous states allow to tune the light transmission through an adjacent photonic waveguide by switching between those configurations. However, mature in-memory computing systems require to tune weights, represented by such transmission states, precisely and reproducibly. To this end, we create electro-optical phase change devices with electrical heaters based on nanometer-thin nanocrystalline graphite, which shows low-loss and can be produced in a simple graphitization process. A PCM is placed directly above stripes of graphite crossing the waveguide. Precise and reproducible tuning of the transmission state is achieved by switching individual, nanoscopic PCM pads fully, avoiding partially crystalline states. Gradual adjustments of the transmission can be achieved by configuring the states of a series of PCM pads with varying size. This way, a limited number of pads can still yield high-resolution weights.

HL 13.16 Mon 15:00 Poster E

**Nanoscopic electrical heaters for mixed-mode in-memory computing with phase change materials** — •Nishant Saxena[1], Niklas Vollmar[1], Ivonne Bente[2], Frank Brückerhoff-Plückelmann[2], Wolfram Pernice[2,3], and Martin Salinga[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Physical Institute, University of Münster, Heisenbergstraße 11, 48149 Münster, Germany — [3]Kirchhoff Institute for Physics, University of Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

In contrast to von-Neumann processors, in-memory computing systems avoid data movement between the processing unit and memory and are therefore fundamentally more efficient. In particular, matrix-vector multiplications on crossbar arrays of photonic waveguides can be performed with extremely high throughput and low energy consumption. A promising approach uses phase change devices to represent the matrix elements. Depending on the phase of the material, a variable fraction of the incoming light is transmitted. We show the realization of mixed-mode phase change devices for in-memory computing on a silicon-on-insulator platform. Their state is written with heating supplied by electrical PIN diodes, which locally heat up individual pads of phase change material on a waveguide. By switching of separate, nanoscopic phase change pads, this scheme enables a reproducible tuning of transmission states with high resolution. The foundry-fabricated devices allow for large-scale integration in mixed-mode integrated circuits with feedback between the photonic and electronic parts.

HL 13.17 Mon 15:00 Poster E

**Theoretical characterization of lead tungstate (PWO-II) crystal structure for improved electromagnetic calorimetry** — •Ather Ahmad[1], Kai-Thomas Brinkmann[1], and Simone Sanna[2] — [1]II. Physikalisches Institut, Gießen, Germany — [2]Institut für Theoretische Physik, Gießen, Germany

Fast response, high density and radiation hardness make lead tungstate (PbWO4 or PWO) a well suited scintillator for an electromagnetic calorimeter. Lead tungstate crystals are already used as working material in various experiments, e.g. CMS at LHC in CERN. New generation crystals (PWO-II) with improved properties were developed for the PANDA experiment at FAIR in Darmstadt.

In order to assess the functionality of the calorimeter, we first need to analyse the electronic and optical properties of lead tungstate. To achieve this the determination of the crystal structure of PWO-II is essential. In our work, we calculate Raman spectra for various phases of PWO crystals in the framework of density functional theory (DFT). Subsequently, these calculated spectra can be compared with experimental Raman spectra of our PWO-II crystals, facilitating the identification of its phase.

This project is supported by HFHF and HGS-hire

HL 13.18 Mon 15:00 Poster E

**Searching for Effective Temperature Seebeck Voltage in Nanoscale Organics** — •Anton Kompatscher and Martijn Kemerink — IMSEAM Heidelberg University, Im Neuenheimer Feld 225 69120 Heidelberg

In contrast to inorganics, organic semiconductors usually show a high degree of energetic and structural disorder. While we have relatively good insight into organics as an ensemble of many molecules, the regime of small (few nanometer) length scales, at which relatively few molecules are probed, remains hardly explored. A phenomenon we are especially interested in is the concept of effective temperature wherein a high >10^7 V/m electric field is predicted to generate electron distributions that correspond to much higher temperatures than the lattice temperature. As modeled in a recent publication, the effective temperature should be able to generate exceptionally high Seebeck voltages, which gives us a good option for experimental verification of the theory. In order to generate sufficient field strengths, the use of nanoscale structures, which we fabricate via electron beam lithography, is necessary. The main challenge in analyzing the signal is to separate spurious effects in the experimental system from the Seebeck voltage, which we do by measuring the response to AC voltages and comparing to theoretical predictions. In particular, we exploit the fact that the Seebeck signal should have double the frequency and zero phase lag compared to the input signal. First results are consistent with the generation of finite effective temperatures, which would constitute the most direct proof of the concept so far.

HL 13.19 Mon 15:00 Poster E

**Theoretical insights into enhanced thermoelectric properties of TTT2I3 and TTT(TCNQ)2 organic nanostructured crystals** — •Ionel Sanduleac and Silvia Andronic — Technical University of Moldova, Stefan cel Mare ave. 168, MD-2004, Chisinau, Republic of Moldova

We present a detailed analysis of the thermoelectric properties exhibited by crystals of TTT2I3, which manifests p-type behavior, and TTT(TCNQ)2 being an n -type conductor. These crystals have been shown to exhibit tunable thermoelectric properties through manipulations of the stoichiometry of charge carriers and impurity concentrations [1]. Crystals of TTT2I3, characterized by a layered structure of alternating tetrathiotetracene and iodide layers, demonstrates efficient charge transport along the main crystallographic axis. Similarly, TTT(TCNQ)2 shares the internal structure of TTT2I3, but with electric conductivity provided by electrons along the TCNQ chains. For this study, we developed a theoretical model, considering electron-phonon interactions and impurity scattering, to analyze transport and thermoelectric properties. The kinetic equation is derived using two-particle retarded Green functions. Electrical conductivity, Seebeck coefficient, thermoelectric power factor, and thermoelectric figure-of-merit were calculated numerically, as function of charge carrier concentrations, temperatures, and impurity concentrations. This study contributes to the understanding of organic thermoelectric materials and their potential role in sustainable energy applications.

[1] I. Sanduleac, et.al.: J. Appl. Physics, 126(17), (2019).

HL 13.20 Mon 15:00 Poster E

**Quantum-chemical calculations of structure, electronic prop-**

**erties, and spectra of neat PBDB-T:ITIC heterojunctions** — Montassar Chaabani[1], Samir Romdhane[1], 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, Tunis, Tunisia — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

In order to overcome the short-comings of polymer:fullerene heterojunctions in organic solar cells, an exchange of the fullerene by other organic molecules, e.g. ITIC has been proposed. In this context, we simulate the structural, electronic and optical properties of PBDB-T:ITIC interfaces quantum-chemically. We constructed oligomers in various conformations in order to represent a segment of the copolymer PBDB-T as well as three conformers of ITIC. These were combined to dimers in either parallel and T-shaped arrangement, and optimized in DFT calculations utilizing the B3LYP-GD3 functional, which considers the Van der Walls interaction semi-empirically. By comparing the MO-energies of the optimized PBDB-T oligomers, ITIC conformers, and dimers, we classified the resulting heterojunctions. Furthermore, we calculated the excited states of the dimers by TD-DFT in order to determine the exciton binding energies and to distinguish charge transfer from excitonic states. Eventually, we provide some indications, to the influence of the PBDB-T:ITIC interface design on the photovoltaic performance.

HL 13.21 Mon 15:00 Poster E

**Effect of trap states on the performance of organic photodetectors** — •Anncharlott Kusber, Jakob Wolansky, Karl Leo, and Johannes Benduhn — Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

In recent years, the scientific community has increasingly investigated novel semiconductors for solar energy conversion. Recently, this field has seen rapid development, and, for example, organic solar cells achieve power conversion efficiencies close to 20 %. Additionally, similar systems have been employed in organic photodetectors (OPDs), showing very competitive specific detectivities $D^* > 10^{13}$ Jones. However, these OPDs, operated under reverse bias, are still limited due to the shot noise, which is proportional to the high dark reserve current [1]. Therefore, a complete understanding of the dark reverse current is necessary. Recent research has revealed a negative impact of mid-gap trap states on the reverse dark current in OPDs [1]. To understand this impact, studies investigated the influence of charge-transfer excitons and trap states using ultrasensitive external quantum-efficiency measurements as well as impedance spectroscopy. We use the techniques as mentioned above on a model system where we intentionally introduce trap states within the active layer. We find a clear trend between the device performance and the presence and quantity of trap states. [1]: Kublitski, Jonas, et al., Nature Communications 12.1 (2021): 551.

HL 13.22 Mon 15:00 Poster E

**Shear-coated highly-smooth ion gels as dielectrics in ion-gated organic field effect transistors** — Jonathan Perez Andrade[1,2], Angelika Wrzesińska-Lashkova[1,2], Anupam Prasoon[1,3], Felix Talnack[1], •Yulia Krupskaya[2], Xinliang Feng[1,3], Yana Vaynzof[1,2], Mike Hambsch[1], Bernd Büchner[1,2], and Stefan C. B. Mannsfeld[1] — [1]Dresden University of Technology, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [3]Max Planck Institute for Microstructure Physics, Halle (Saale), Germany

We have developed a straightforward method to produce ion gels with surface roughness at the nanometer scale using a shear-coating process and employed these gels as ultra-smooth dielectric substrates in organic field effect transistors (OFET). The exceptional smoothness of the gels allowed us to grow polycrystalline films of C8-BTBT (2,7-Dioctyl[1]benzothieno[3,2-b][1]benzothiophen) and C10-DNTT (2,9-Didecyldinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene) and to evaporate metal contacts on their surface. Besides that, the shear-coating process increased the ion concentration at the gel's surface leading to a remarkably high capacitance up to 10.1 $\mu$F/cm$^2$. The obtained ion-gel-based OFET showed very good characteristics with low hysteresis and maximum charge carrier mobility of 0.54 cm$^2$/V/s and 0.27 cm$^2$/V/s for C10-DNTT and C8-BTBT devices, respectively. These results demonstrate the significant potential of using shear-coated ion gels in fabrication of high quality OFET.

HL 13.23 Mon 15:00 Poster E

**Study of the metal-insulator transition of Peierls type in quasi-one-dimensional organic crystals.** — •Silvia Andronic and Ionel Sanduleac — Technical University of Moldova, Stefan cel Mare ave. 168, MD-2004, Chisinau, Republic of Moldova

The purpose of the current study is to investigate the metal-insulator transition occurring in quasi-one-dimensional organic crystals (Q1D) of TTF-TCNQ, TTT(TCNQ)2 and TTT2I3. The use of these materials brings several advantages, including cost-effectiveness, environmental safety and relatively inexpensive manufacturing processes. Additionally, the growing interest in certain Q1D organic crystals is attributed to their high electrical conductivity. The research employs a 3D approximation method and introduces a physical model that incorporates two significant electron-phonon interaction mechanisms, one akin to the deformation potential and the other exhibiting polaron characteristics. We also account for scattering on defects, a crucial factor in explaining the transition. Using the random phase approximation and Green functions method, we calculate the phonon polarization operator and the renormalized phonon spectrum at different temperatures and various dimensionless Fermi momentum (kF) values. The results suggest that the transition demonstrates Peierls-type characteristics, and the critical temperature linked to the Peierls transition is identified. Furthermore, we observed that the Peierls critical temperature significantly decreases as the carrier concentration increases. The impact of lattice distortion on the dispersion of renormalized acoustic phonons is also considered.

HL 13.24 Mon 15:00 Poster E

**Single molecule spectroscopy of emitters in hexagonal boron nitride** — •Osama Farooqui and Klas Lindfors — Department of chemistry, University of Cologne, Greinstr.4-6, D-50939, Cologne, Germany

The interaction of light with atoms or molecules is indispensable in the examination of materials for potential use in the development of high-speed communication devices [1]. The primary objective of this project is to observe light emission and absorption within heterostructures comprised of two- and one-dimensional materials, as well as single emitter molecules.

Previously, investigations were conducted on individual triisopropylsilyl pentacene (TIPS-pentacene) molecules on a glass substrate using single molecule spectroscopy. To address the challenge of molecular stability, hexagonal Boron Nitride (hBN) is employed to encapsulate emitter molecules, thereby preventing chemical reactions with the surrounding environment. Initial data from time traces of TIPS-pentacene molecules encapsulated in hBN flakes indicate that these molecules do not undergo photobleaching over a one-hour period at room temperature. However, rapid photoblinking is observed in the time traces of the molecules. The cause of this fast photoblinking is speculated to be the interaction of the molecules with nearby two-level systems, potentially associated with hBN flakes.

Reference

[1] Toninelli, C. et al. Single organic molecules for photonic quantum technologies. Nat. Mater. 1*14 (2021).

HL 13.25 Mon 15:00 Poster E

**Optimisation of the surface structure of a Pt/TiOx sensor for low concentrations of hydrogen** — •Anastasija Scherer, Marvin Rauhut, Thomas Heinzel, and Mihai Cerchez — Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

Mesoporous TiOx based hydrogen sensors are highly sensitive also at ppm concentrations [1], however, the results are highly dependent on the parameters of the TiOx internal structure, like defect density or internal surface-to-volume ratio. The sensors are produced by anodisation of industrial grade Ti foil in solution of sulfuric acid [2]. The process leads to the formation of a TiOx thin layer of thickness of the order of micrometers, and surface aspect varying between sandy and spongeous, with a characteristic mesh size of the order of 100 nm. This is controlled by the voltage used during the anodisation process as well as subsequent thermal annealing. Measurements of the sensing capability will be presented. [1] Appl. Phys. Lett. 103, 033522, 2013 [2] Metals 8, 386, 2018

HL 13.26 Mon 15:00 Poster E

**Sensing acetaldehyde using Pt/TiOx sensors** — •Marvin Rauhut, Anastasija Scherer, Thomas Heinzel, and Mihai Cerchez — Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

The photocatalytic decomposition has been shown to be the most promising route to air purification for volatile organic compounds, both

at TiOx [1] and Pt/TiOx [2] catalyst surfaces. Here, a vertical structure formed by a thin Pt layer on a mesoporous TiOx film with high density of oxygen vacancies is used as a sensor for acetaldehyde. While first results are encouraging, this presentation will show the progress on tuning the surface structure to maximise sensitivity to acetaldehyde, measured as the change of the resistance of the sensor during the exposure to various concentrations of acetaldehyde. [1] Catalysts, 10, 1464, 2020 [2] J. Catal., 179, 171, 1998

HL 13.27 Mon 15:00 Poster E

**Heteroepitaxial Growth of Ge-doped $\gamma$-$Ga_2O_3$ Ultrawide Bandgap Semiconductor Thin Films on (100) $MgAl_2O_4$ Substrates by Pulsed Laser Deposition** — •Jingjing Yu, Sijun Luo, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth System Sciences, Universität Leipzig, 04103 Leipzig

$\gamma$-$Ga_2O_3$ is a defective cubic spinel metastable phase of ultrawide bandgap gallium oxides. In order to compensate the volatile loss of Ge components, a Ge-rich target with a Ge:Ga atomic ratio of about 17:1 was used to grow (100)-oriented $\gamma$-$(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin films on cubic spinel (100) $MgAl_2O_4$ substrates using pulsed laser deposition. The $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin films are fully-strained, and the in-plane orientation relationships are [010] $(Ga_{1.73}Ge_{0.27})O_3$ // [010] $MgAl_2O_4$ and [011] $(Ga_{1.73}Ge_{0.27})O_3$ // [011] $MgAl_2O_4$. The 215 nm thick (100) $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin film shows the rocking curve of (400) reflection with a full width at half maximum (FWHM) of about 0.022 degrees ( 80 arcseconds). The electrical properties of $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin film were evaluated by temperature-dependent Hall measurements. The resistivity of film decreases dramatically from about 30000 Ω cm to 6 Ω cm as temperature increases from 125 to 350 K. The electron carrier concentration of thin film increases from 2.1 x $10^{14}$ $cm^{-3}$ at 125 K to 2.6 x $10^{17}$ $cm^{-3}$ at 350 K with an estimated activation energy of about 117 meV. While the Hall electron carrier mobility gradually increases from 0.4 to 4.1 $cm^2$ $V^{-1}s^{-1}$ as the temperature increases from 125 to 350 K.

HL 13.28 Mon 15:00 Poster E

**Screening of different p-type materials for pn-heterojunctions on $\alpha$-$Ga_2O_3$**

— •Paul Bokemeyer, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Germany

With a 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], the corundum $\alpha$-phase of $Ga_2O_3$ is highly interesting for high power applications. Schottky barrier diodes have been shown to exhibit high rectification ratios [3] and the first isostructural *pn*-diodes using $\alpha$-$Ir_2O_3$ as p-type material have been demonstrated [4]. We evaluate the electrical properties of various heterojunction diodes on $\alpha$-$Ga_2O_3$:Sn grown by pulsed laser deposition (PLD). Room temperature deposited ZCO (PLD), NiO (PLD) and CuI (sputtering) were used as $p^+$-type materials. Thereby NiO as well as CuI enable the fabrication of fully transparent devices in the visible spectral range. High current rectification ratios of 6.3 (ZCO), 3.9 (NiO), and 4.6 (CuI) orders of magnitude at ± 3V were achieved.

[1] A. Hassa *et al.*, J. Phys. D: Appl. Phys. 54 223001 (2021)
[2] M. Biswas and H. Nishinaka; APL Materials 10, 060701 (2022)
[3] S. Köpp *et al.*, J. Vac. Sci. Technol. A 41, 043411 (2023)
[4] S. Kan *et al.*; Appl. Phys. Lett. 113, 212104 (2018)

HL 13.29 Mon 15:00 Poster E

**Cation segregation in an $(In,Ga)_2O_3$ thin film library beyond the miscibility limit of the bixbyite structure** — •Sandra Montag[1], Daniel Splith[1], Max Kneiss[1], Marius Grundmann[1], Javier Garcia Fernandez[2], Øystein Prytz[2], and Holger von Wenckstern[1,2] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo, Norway

The transparent semiconductors $In_2O_3$ and $Ga_2O_3$ crystallise in different polymorphs. Hence, a phase change occurs in the alloy system of $(In_{1-x}Ga_x)_2O_3$, grown in bixbyite cubic structure at low $x$. To observe this change, a material library of thin films with $0.1 \leq x \leq 0.64$ was fabricated by discrete combinatorial synthesis on r-plane sapphire substrates using pulsed laser deposition. The samples crystallize in the bixbyite phase for $x \leq 0.35$, as revealed by X-ray diffraction. However, lattice constant and absorption edge energy systematically decrease and increase, respectively, with increasing Ga content only up to $x = 0.2$. For higher Ga admixtures, both saturate. In addition, a significant change in surface morphology occurs at $x \sim 0.2$. Transmission electron microscopy examinations of selected samples show a homogeneous incorporation of $Ga_2O_3$ into cubic $In_2O_3$ for $x = 0.11$, while a segregation of Ga-rich and In-rich regions can be seen for higher $x$. In a sample with $x = 0.35$, the Ga-rich regions exhibit a preferred orientation, which has been shown to result from a correspondingly faceted In-rich bixbyite layer at the substrate-thin film interface.

HL 13.30 Mon 15:00 Poster E

**PLD Deposition of the transistion metal sesquioxides $\alpha$-$Ti_2O_3$ and $\alpha$-$Cr_2O_3$** — •Lorenz Köhnlein, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Deutschland

Corundum phase sesquioxides like $Ti_2O_3$ and $Cr_2O_3$ are ideally suited for band gap engineering within $\alpha$-$Ga_2O_3$-based ternary alloys to design wavelength-selective optoelectronic devices. It has been shown that rhombohedral $Ti_2O_3$ has a narrow-bandgap of $\approx$ 0.1 eV [1]. Therefore, Ti could be used as a band gap modifier for $\alpha$-$Ga_2O_3$ to tune the bandgap between 0.1 eV and 5.3 eV [2].

We present physical properties of PLD-grown $Ti_2O_3$ and $Cr_2O_3$ thin films, deposited on m-, a- and c-plane $Al_2O_3$ substrates as well as on $\alpha$-$Ga_2O_3$ buffer layers at various growth temperatures, atmospheres and pressures. Hall-effect and XRD measurements were used to investigate the electrical and crystalline properties. A strong dependence of the crystal phase formation on the background gas and pressure was observed. Argon atmosphere faciliated the growth of $Ti_2O_3$, whereas oxidisation to $TiO_2$ occured during the deposition in oxygen atmospheres even at low pressures.

HL 13.31 Mon 15:00 Poster E

**Reduction of droplet density for pulsed Laser Deposition of functional oxides** — •Jonas Elz, Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Pulsed laser deposition is a highly flexible and reproducible technique for epitaxial growth of high quality thin films [1]. Two major problems occurring for certain target materials are the formation of droplets on the substrate and the increasing surface roughness of the target during laser ablation that may cause a change of the expansion direction of the plasma plume towards the direction of the incident laser beam [2, 3]. Thin films containing droplets are undesirable for device applications.

In this work, we present means for a significant reduction of the density of droplets for copper oxide targets using a shadow mask (so-called eclipse) between target and substrate. The effect of the laser fluence incident on target on its surface roughness and the change of plasma plume expansion direction during deposition will be presented in detail.

[1] David P. Norton, in Pulsed Laser Deposition of Thin Films, Wiley, Hoboken (2007)
[2] S. Fahler et al., Appl. Surf. Sci. 109/110 433-436 (1997)
[3] C. Doughty et al., Appl. Phys. Lett. 66, 1276-1278 (1995)

HL 13.32 Mon 15:00 Poster E

**The influence of Band bending on valence band offsets determined by Kraut's method: Modeling and experiment for polar-discontinuity doped $LaInO_3$/$BaSnO_3$** — •Georg Hoffmann[1], Aysha A Riaz[2], Anna Regoutz[2], Oliver Brandt[1], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Chemistry, University College London , London, UK

Two-dimensional electron gases (2DEGs) in $LaAlO_3$/$SrTiO_3$ heterostructures due to polar discontinuity have brought huge attention to perovskite oxides [1]. For $LaInO_3$/$BaSnO_3$ heterostructures, a predicted conduction band offset (CBO) of 1.6 eV confines a charge carrier density of up to $2\times10^{14}$ $cm^{-2}$ in the quantum well at the $BaSnO_3$ side [2], while room temperature mobilities are higher by one order of magnitude compared to $SrTiO_3$ based 2DEGs. To determine the CBO considering interfacial band bending the related valence band offset (VBO) is determined by Kraut's method using x-ray photo electron spectroscopy (XPS) [3].

We developed a model that predicts XPS core-level (CL) shape and shift for given band profiles and thus related VBO correction.

Synchrotron-based XPS data are interpreted with this model to determine band bending and VBO at the $LaInO_3/BaSnO_3$ interface.

[1] J. Mannhart, et al., MRS bulletin 33, 1027-1034 (2008). [2] W. Aggoune, and Claudia Draxl, npj Computational Materials 7, 174 (2021). [3] E. A. Kraut, et al., Phys. Rev. Lett. 44, 1620 (1980).

HL 13.33 Mon 15:00 Poster E

**Investigating the iodoplumbate complex evolution of perovskite solution during spin coating via UV-VIS in-situ spectroscopy** — •Maximilian Spies, Simon Biberger, and Anna Köhler — University of Bayreuth, Bayreuth, Germany

We investigated the precursor solution for the fabrication of $MAPbI_3$ perovskite thin films via UV-VIS absorption spectroscopy during the spin coating process (in-situ). The iodoplumbate complexes present in this precursor solution absorbe light in the UV range, providing insights into the precursor chemistry that is crucial for the formation of the final perovskite film. Since these iodoplumbate complexes are very sensitive to their environment and can alter their coordination considerably when changing parameters like the solvent or concentration, we conducted an in-situ study during the critical phase before the nucleation in order to get a deeper insight into the formation dynamics of neat perovskite thin films. We find that an absorption peak, commonly stated to originate from the $PbI_3^-$ complex, shifts to lower energies with respect to time during spin coating, indicating a growth of the electronic system. The amount of this red shift depends on the precursor concentration and the composition of the solvent in use.

HL 13.34 Mon 15:00 Poster E

**Mask and Plate Metallization for High-Efficiency Solar Cells** — •Maral Ghanbari[1,2], Jörg Schube[1], Tadeo Schweigstill[1], Gabriele Mikolasch[1], Roman Keding[1], and Andreas W. Bett[1,2] — [1]Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstraße 2, 79110 Freiburg — [2]University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg

The pursuit of higher conversion efficiency in solar cells is a central objective in photovoltaic manufacturing. Narrowing fingers is one option due to a significant decrease in shading losses. Through precise control of finger dimensions, we aim to enhance solar cell conversion efficiency, specifically for perovskite-silicon tandem solar cells. This study introduces a potential remedy, involving mask and plate metallization technology for perovskite-silicon tandem solar cells. The technique, detailed here, comprises three stages: masking, electroplating, and mask stripping. In the masking phase, hotmelt ink is applied to the substrate via inkjet printing, creating a wax-based phase-change mask with open areas. In the electroplating phase, metal contacts are precisely positioned on these areas, enabling silver-free metallization. In the final stage, the mask can be easily removed using isopropyl alcohol. The primary aim of this study is to develop and understand the inkjet printing process for producing a mask with the narrowest openings, aiming to reduce shading-related losses with metal contacts achieving a width of less than 20 micrometres.

HL 13.35 Mon 15:00 Poster E

**Strain effects on the electronic structure of Cs-based metal halide perovskites** — •Freerk Schütt[1], Ana M. Valencia[1,2], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg — [2]Humboldt-Universität zu Berlin und IRIS Adlershof, Berlin

Metal-halide perovskites (MHPs) are promising materials for photovoltaics, but fundamental studies on their structure-property relationships are still needed to exploit their full potential. Using density-functional theory, we analyze the effects of compressive and tensile strain between -3% and 3% in $CsXI_3$ with X = Sn, Pb, in order to provide fundamental insight into the influence of lattice deformation on the structural and electronic properties of these materials, particularly related to the modulation of the band gap. These underlying structural changes, notably the significant distortion of the characteristic octahedra, are larger with Sn than with Pb, likely due to the larger flexibility of Sn-based MHPs over their Pb-based counterparts. Our results provide useful insight for tuning electronic properties and improving stability through strain-engineering of MHPs.

HL 13.36 Mon 15:00 Poster E

**Temperature-induced limitation of charge carrier mobility in perovskite absorbers and its influence on recombination** — •Patrick Dörflinger, Philipp Rieder, and Vladimir Dyakonov — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

The charge carrier mobility $\mu$ is a crucial parameter in semiconductors. Together with the lifetime, it quantifies the diffusion length of the charge carriers. Moreover, its temperature-dependent power-law $\mu \propto T^{-\gamma}$ provides information about the predominant scattering mechanism that limits mobility at a certain temperature. For lead-halide perovskites $\gamma$ values of $\approx 1.5 - 3$ are observed at room temperature, which are related to pronounced displacements of the lead-halogen bonds due to the rather mechanically soft lattice.[1] More importantly, this scattering mechanism dominates at elevated temperatures and severely restrics charge carrier mobility, an effect relevant for photovoltaic applications.

For this reason, we systematically investigated the charge carrier decay, mobility, and power-law behavior between 80K and 360K using time-resolved microwave conductivity (TRMC). We find a correlation between the scattering mechanism and the recombination behavior of the charge carriers in methylammonium lead triiodide. Furthermore, by substitution of the A-site cation and halide anion we quantify the predominant scattering mechanism of different organic/inorganic lead halide perovskites, which exhibit different temperature dependencies.

[1] Dörflinger et al., *Adv. Sci.* **2023**, 2304502.

HL 13.37 Mon 15:00 Poster E

**Circular Dichroism and Polarized Emission in Bismuth doped Pyridyl-ethylamine Lead Iodide 2D Perovskites** — •Henrik Spielvogel[1], Jan-Heinrich Littmann[1], Philip Klement[1], Lukas Gümbel[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

The incorporation of chiral organic cations into lead halide perovskites enables the resulting 2D system to exhibit properties such as chiroptical activity and chirality-induced spin selectivity allowing the generation and detection of circularly polarized light. Doping and alloying serve to modify and enhance the properties and performance of such materials. When doping with cations of differing charge to the constituting $Pb^{2+}$ ions, defect creation is inevitable and the effects on chiroptical activity are not yet known due to complex structure-property relationships and experimental limitations.

Here, we present $Bi^{2+}$-doped pyridyl-ethylamine lead iodide as a model compound for doped chiral lead iodide perovskites. Through polarization-resolved spectroscopy, we characterize the relationship between circular dichroism and structural factors. This analysis offers valuable insights for designing new materials with high chiroptical activity.

HL 13.38 Mon 15:00 Poster E

**Circular Dichroism and Polarized Emission in Bismuth doped Methylbenzylamine Lead Iodide 2D Perovskites** — •Jan-Heinrich Littmann[1], Henrik Spielvogel[1], Philip Klement[1], Lukas Gümbel[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Organic-inorganic metal-halide perovskites are intriguing research materials due to their remarkable semiconductor properties and the potential applications ranging from photovoltaics to solid-state lighting and detectors. The incorporation of chiral organic cations into lead halide perovskites showcased chiroptical activity as well as chirality-induced spin selectivity. These characteristics hold promise for applications in emitters and detectors of circularly polarized light. Performance can be further boosted via doping and alloying. However, heterovalent doping using $Bi^{3+}$ is currently not fully understood due to intricate structure-property relationship. We investigate a $Bi^{3+}$-doped methylbenzylamine lead iodide model compound specifically on circular dichroism and emission polarization. Additionally, the substitution of $Pb^{2+}$ by $Bi^{3+}$ introduces free charges that lead to additional defects and dopants. Our objective is to uncover how structural factors impact circular dichroism, aiming to provide insights for designing materials with elevated chiroptical activity.

HL 13.39 Mon 15:00 Poster E

**Exploring anharmonicity in metal halide double perovskites using machine-learned ACE potentials** — •Mattis Gossler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Metal halide perovskites (MHPs) have gained much attention for their exceptional photo-electrical properties, making them ideal for photovoltaic applications. Seeking eco-friendly alternatives to traditionally lead-based MHPs, double-cation perovskites $A^{I}_{2}M^{I}M^{III}X_{6}$ offer fine-tuned photo-electrical properties through their variable composition.

MPHs are softer compared to other inorganic semiconductors, displaying significant structural fluctuations at room temperature. Understanding their electronic and structural properties involves anharmonic vibrational modes, best explored through *ab initio* molecular dynamics (AIMD). To overcome the severe simulation limitations of AIMD, we employ an on-the-fly active-learning workflow to train an atomic cluster expansion (ACE) machine-learned interatomic potential with minimal human intervention. The capabilities of the generated ACE potential are then tested to investigate structural and dynamic properties of the double perovskite $Cs_2AgBiCl_6$ from the CANBIC family at elevated temperatures, which are still ambiguous from experimental data.

HL 13.40 Mon 15:00 Poster E

**Excitonic and optical properties of a novel halide-based double perovskite from ab-initio many body techniques** — •Manaswita Kar, Maria Hellgren, Michele Casula, and Benjamin Lenz — Sorbonne Univesité, Paris, France

Halide perovskites have proved to be promising candidates for next-generation photonics applications, including both classical and quantum emission. The exceptional excitonic and optical properties of this class of materials are in particular in focus in their quantum-confined regime. In this study, we investigate the optical and excitonic properties of a novel halide-based double perovskite, which was first predicted by machine learning and subsequently validated by synthesis and characterization of quantum dots. Here, we characterize the optical properties of the bulk phase through theoretical simulations. We employ many-body perturbation theory (GW) and Bethe-Salpeter equation techniques to study its excitonic properties, which are not captured within standard density functional theory.

HL 13.41 Mon 15:00 Poster E

**Understanding the Methylammonium Chloride-Assisted Crystallization for Improved Performance of Lead-Free Tin Perovskite Solar Cells** — •Daniele Cuzzupè — University of Konstanz, Konstanz, Germany

In the quest for perovskite materials with reduced toxicity, Sn perovskites are emerging. However, they suffer from material instability and rapid crystallization, leading to high defect densities in the films. In this work, the methylammonium chloride (MACl)-assisted crystallization as a route to improve stability and optoelectronic quality of quasi 2D/3D PEA0.08FA0.92SnI3 perovskite is demonstrated. For an optimal additive amount (10 mol%), a 37% increase in power conversion efficiency is found. Notably, MACl enhances the films' stability, evidenced by temporal PL tracking. Understanding the effect of MACl addition in this system is interesting for the pursuit of efficient and stable tin-based devices. The investigations show that MACl addition causes a shift in the optical bandgap and improves morphology, indicating effects in the bulk crystal structure. X-ray photoelectron spectroscopy confirms the presence of Cl on the surface, but no indication of MA+ is found. Intriguingly, UV photoelectron spectroscopy shows pronounced changes in the density of states. For the first time, it is shown that MACl promotes the formation of a two-dimensional layer via the surface accumulation of PEA+. The MACl additive lowers the absorber's ionization energy, possibly facilitating hole extraction. Overall, this work highlights a facile route to control the crystallization of Sn perovskites.

HL 13.42 Mon 15:00 Poster E

**Photoelectron spectroscopy and in-situ time-resolved photoluminescence for the characterization of thin film solar cells** — •Philine Stötzner, Alexander Stauffenberg, Torsten Hölscher, Roland Scheer, and Stefan Förster — Martin-Luther Universität Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany

Alkaline doping plays an important role in improving the efficiency of chalcogenide solar cells based on $Cu(In,Ga)(Se,S)_2$ (CIGS). By X-ray photoelectron spectroscopy (XPS) performed in ultrahigh vacuum (UHV), we identified the segregation of sodium towards the absorber surface after a controlled exposure to light and various gases. It leads to a degradation of uncoated absorbers that persists even after completion of the whole solar cell [1]. The reduction of the charge carrier lifetime has been confirmed by ex-situ time-resolved photoluminescence (TRPL). Here, we present a setup that combines XPS and in-situ TRPL in UHV accompanied by UPS to study the valence band electronic structure. The experimental setup contains a high-pressure gas cell for exposure to ultra-pure gases or air, a controlled illumination, and alkali dispensers. This setup is perfectly suited to trace back chemical surface modifications and changes in the charge carrier mobilities and electronic properties to a distinct environmental stimulus. Thus, it is not limited to CIGS but also for other absorber materials like organo-metal halide perovskites.

[1] T. Hölscher et al., Progress in Photovoltaics 26 (11), (2018)

HL 13.43 Mon 15:00 Poster E

**Low temperature photoexcitation dynamics in triple cation lead halide perovskites** — •Alexander Schauerte[1], Isabel Allegro[2], Anton Krüger[1], Ian Howard[2], Uli Lemmer[2], and Marina Gerhard[1] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, Germany

Hybrid perovskites are a promising class of materials not only for cheap and efficient solar cells, but they also show a huge potential for lasing applications. In both cases, the charge carrier dynamics is of great interest.

Here, we study the recombination dynamics of the triple cation lead halide perovskite $Cs_{0.1}(MA_{0.17}FA_{0.83})_{0.9}Pb(I_{0.84}Br_{0.16})_3$ using time-resolved photoluminescence spectroscopy. The combination of spectrally and spatially resolved measurements allows us to explore the relaxation pathways of carriers and their spatial diffusion on the picosecond time scale.

At low temperatures, the diffusion at early times is enhanced compared to higher temperatures, but saturates within a nanosecond. Moreover, the low-temperature spectra reveal a red-shift over time, particularly below approximately 70 K, indicating the population of energetically relaxed and more localized states. We attribute the dispersive dynamics at low temperatures to the absence of dynamic disorder, which mitigates self-trapping effects at early times, but leads to the population of localized emissive tail states at later times, unraveling the underlying static disorder.

HL 13.44 Mon 15:00 Poster E

**Nanoparticle and polymer based optical coating for stability and thermal management of perovskite solar cells** — •Steffen Richter, Sema Sarisözen, Sercan Özen, Frank Jaiser, Thomas Hultzsch, and Felix Lang — Radiation-Tolerant Electronics with Soft Semiconductors , University of Potsdam, Germany

Photons with energies outside the band gap are not only not utilized, but often decrease performance and stability of perovskite solar cells. Harsh UV light can trigger various degradation mechanisms, while IR light leads to excessive heating.

Commercial protections are usually quite expensive. To increase the stability, reduce heat and improve performance with an affordable and simple approach we aim at introducing an optical coating containing various nanoparticles embedded into an encapsulating polymer.

Our first results show that indium tin oxide nanoparticles absorb and reflect near infrared light, while (aluminum doped) zinc oxide nanoparticles absorb ultraviolet radiation and downshift the latter to an emission in the visual spectrum. Further, PDMS as an embedding polymer acts like a natural anti reflection layer. Bioinspired structuring of the surface with rose petals decreases reflectance and increases transmittance additionally. In literature PDMS is used for radiative cooling because of its conversion of heat to emission in higher infrared wavelengths which could reduce the cell temperature even further.

In this poster we will present detailed transmission and reflection spectra as well as evidence of downshifting. Further, we will show how the optical coating will affect device performances.

HL 13.45 Mon 15:00 Poster E

**Ultra-thin subwavelength detection of polymer layers using highly-doped n-Ge plasmonic antenna in the THz range** — •Elena Hardt[1], Carlos Alvarado Chavarin[1], Julia Flesch[2], Oliver Skibitzki[1], Romualdo Varricchio[3], Alessandra di Masi[3], and Giovanni Capellini[1,3] — [1]IHP - Leibniz Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]University of Osnabrueck, Barbarastrasse 11, 49076 Osnabrueck, Germany — [3]Department of Sciences, Università Roma Tre, Viale G. Marconi 446, 00156, Roma, Italy

The advatanges of THz instrumentation for biosensing is based on the

high sensitivity to polar substances and on very low energy photons of the THz range. Thus, recent improvements in THz sources and detectors allow label-free, reliable measurements of biomolecules. LSPR is an ideal concept to enhance the spectroscopy signal and to improve the sensitivity. In this work, we investigate the sensitivity of highly n-doped Ge plasmonic THz antennas realized on Si and SOI substrates in presence of ultra-thin subwavelength polymer layers. The antenna response to the well-known electrostatic layer-by-layer deposition is investigated by observing the shift of the LSPR in the THz spectra. 5, 15 and 22 layers of poly-(allylamine)PAN/poly-(acrylic acid)PAA show a linear response. By using an optimized antenna design relying on low losses SOI substrates, we detect resonance spectral shifts as large as 14.5 GHz in response to 22 PAN/PAA layers of a few nm-thickness. We believe that this result could pave the way to a low-cost CMOS compatible biosensing platform.

HL 13.46 Mon 15:00 Poster E

**THz Spectroscopy on $Bi_2Se_3$** — •Debankit Priyadarshi[1,2], Amit Haldar[1], Sunil S. Kushvaha[3], Manfred Fiebig[2], and Shovon Pal[1] — [1]School of Physical Sciences, National Institute of Science Education and Research, HBNI, Jatni, India. — [2]Department of Materials, ETH Zurich, Zurich, Switzerland. — [3]CSIR-National Physical Laboratory, New Delhi, India.

Topological insulators (TI) have come up as an important condensed matter system showing exotic metallic surface states protected by their topology and time reversal symmetry. The investigation of the conductivity of these surface states is difficult with traditional electrical techniques due to contributions from the free carriers in the bulk and the quantum well states to the total conduction. Terahertz (THz) spectroscopy is an emergent field in probing the conduction properties of these surface states due to the low photon energies (meV) of the THz radiation. Our measurements show contributions from Drude-like charge carriers and two Lorentz oscillator-like resonances to the conductivity of the $Bi_2Se_3$. The oscillator responses are attributed to the bulk-phonon resonance and inter-sub-band transitions in the quantum well states. The Drude response is expected to have contributions from the surface state carriers, 2D electron gas present on the quantum well states and free carrier states of the bulk. Going into the relaxation dynamics of these carriers by doing pump-probe measurements would reveal the exact contribution of the surface state carriers to the conductivity.

HL 13.47 Mon 15:00 Poster E

**Ultrafast THz Engineering of Semiconductor Photoluminescence** — •Maximilian Frenzel, Joanna M. Urban, Michael S. Spencer, Martin Wolf, and Sebastian F. Maehrlein — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Exploring the interaction between THz radiation and semiconductor photoluminescence (PL) presents a potential avenue for developing future optoelectronic devices and gaining novel insights into ultrafast semiconductor physics. In this work, we employ single-cycle THz pulses (0.5-4 THz) with peak fields exceeding 1 MV/cm to control the PL of a bulk ZnTe semiconductor. We find that THz pulses can quench the total emitted PL by more than 50% at room temperature. In addition to reducing the emission magnitude, the THz pulses also affect the PL's spectral weight, thus allowing the PL to be tailored by the THz fluence. Moreover, we study THz-induced quenching as a function of time delay with respect to the photo carrier injection, which provides a further control knob to tune the emission, whilst also constituting an ultrafast probe for studying the interplay of lattice and carrier dynamics. Our work serves as a systematic study to control the emission and carrier dynamics using THz light and establishes a testbed for future investigations of electron-phonon interactions in emerging semiconductors.

HL 13.48 Mon 15:00 Poster E

**Investigating the stability and electronic properties of CuI (111) polar surfaces** — •Preeti Sharma[1], Silvana Botti[1,2], and Tomáš Rauch[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems of the Research Alliance Ruhr, Faculty of Physics and ICAMS, Ruhr University Bochum, Germany

In recent years, CuI has drawn the attention of many researchers as a most suitable p-type transparent conducting material (TCM) due to its large band gap (3.1 eV), large exciton binding energy (62 meV), and high carrier mobility. Because of these properties, CuI thin films are proposed as prominent candidates for optoelectronics devices such as solar cells, light-emitting diodes, etc. It is crucial to understand the surface properties, like, surface reconstruction, surface energy, and band structure for the development of CuI-based devices. Here, we investigated the stability and electronic properties of Cu-terminated and I-terminated (111) polar surfaces using first principles. A standard slab method cannot be used to calculate the surface energies for polar surfaces. Therefore, we used the wedge structure model and evaluated surface energy for one polar surface without involving its associated surfaces.

HL 13.49 Mon 15:00 Poster E

**Optimisation of pulsed-laser-deposition-grown CuI polariton microcavities** — Kirsty E. McGhee, Lukas Trefflich, Aaron Giess, Marius Grundmann, and •Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Exciton-polaritons are light-matter quasiparticles that possess properties of both excitons and photons, making them of great interest for ultra-low threshold lasers, all-optical circuits, and quantum simulators. Because excitons and photons are both bosons, polaritons are also bosons and, under certain conditions, can undergo a non-equilibrium Bose-Einstein-like condensation. In this work, we discuss our efforts to realise polariton condensation in a microcavity containing copper iodide (CuI), a transparent semiconductor currently of great interest due to its inherent p-type behaviour. We discuss the optimisation of the growth of the CuI layer and of the distributed Bragg reflectors (DBRs), the highly-reflective mirrors used to confine the cavity mode, using pulsed laser deposition. In particular, we have found adhesion problems between CuI and the low-refractive-index dielectrics $Al_2O_3$ and MgO ($n$∼1.7). These adhesion problems disappear when we instead grow the CuI between layers of yttria-stabilised zirconia (YSZ, $n$∼2.1). However, while we demonstrate the presence of exciton-polaritons, we do not see any evidence of polariton condensation at room temperature or cryogenic temperatures, likely due to the low cavity quality factor. In order to enhance this quality factor, further optimisation is required, which will be presented here.

HL 13.50 Mon 15:00 Poster E

**State of the art S/TEM-based strain measurement techniques** — •Laura Niermann[1], Tore Niermann[1], Frederik Otto[1], Rahel Spect[1], Paul Schmiedeke[2], Gregor Koblmüller[2], and Michael Lehmann[1] — [1]Technische Universität Berlin, Berlin — [2]Technische Universität München, München

Strain fields influence the electronic and optical properties of semiconductor materials. (Scanning-) transmission electron microscopy (S/TEM) enables the measurement of strain fields on the nanometer scale. We present results from current S/TEM-based strain measurement techniques on several semiconductor hetero-structures: Dark-field electron holography excels at strain measurements over extended regions within semiconductor devices by analyzing the phase of a single diffracted beam. Alternatively, nano beam electron diffraction enables strain mapping through the acquisition of entire electron diffraction patterns at each scan position. The precision of the latter technique can be further improved upon by means of precession electron diffraction. However, so far these approaches required the strain to be constant along the electron beam. We present new methodologies for evaluating three-dimensional strain variations from a single projection. This is achieved by combining scanning convergent beam electron diffraction (SCBED) patterns or dark field electron holographic tilt series with numerically efficient multi-beam calculations. Additionally, we demonstrate how such combined measurement and modeling approaches even enables a classification of quantum dot shapes.

HL 13.51 Mon 15:00 Poster E

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

A wide band gap of 3 eV at room temperature and its intrinsic $p$-type conductivity[1] render copper iodide (CuI) a promising candidate for the fabrication of transparent heterostructure diodes. However, the often degenerate hole concentration of up to $10^{20}$ cm$^{-3}$[1] of binary CuI impedes the realization of rectifying heterostructures where the depletion layer is located in the CuI. By alloying CuI with Ag, a reduction of conductivity and carrier density was demonstrated for an increasing silver fraction $x$[2]. Additionally, a switch from $p$- to $n$-type conductivity was reported, which enables the fabrication of heterostructure

*pn*-diodes based on silver copper iodide ($Ag_xCu_{1-x}I$)[3].

We present transparent heterostructure diodes based on the ternary alloy $Ag_xCu_{1-x}I$ on different *n*-type back contact layers. $Ag_xCu_{1-x}I$ is deposited by means of reactive co-sputtering of metallic Cu and Ag in an argon and iodide atmosphere. The influence of the back contact layers on the functionality and the rectifying behaviour of the *pn*-junctions is compared and presented.

[1] C. Yang *et al.*, PNAS, 113, 12929-12933, 2016.
[2] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.
[3] J.-H. Cha and D.-Y. Jung, ACS Appl. Mater. Interfaces, 9, 43807-43813, 2017.

HL 13.52 Mon 15:00 Poster E

**Combined Optical and Atomic Force Microscopic Investigation of Type-I CdSe/CdS Dot-in-Rod Particles with Metal Tips** — •Nicklas Giese, Mareike Dittmar, Moritz Wehrmeister, Alf Mews, and Tobias Kipp — Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany

Semiconductor-metal-hybrid nanostructures can split water and produce hydrogen by illumination, such as dot-in-a-rod particles with a charged metal tip. The understanding and control of the charge transfer processes of these particles is crucial for their further development. We investigate hybrid nanostructures consisting of a CdSe-core/CdS-shell with a metal tip attached. Optical characterization is performed by time-resolved single-particle photoluminescence (PL) spectroscopy. Thereby, the attachment of the metal tip can be correlated with the decrease in quantum yield (QY) and PL lifetime of the semiconductor, giving detailed information on charge-carrier separation. We present an all-in-one setup that combines PL spectroscopy to Kelvin probe force microscopy (KPFM) with simultaneous local illumination of the nanostructure. KPFM is based on an atomic force microscope (AFM) with a conductive cantilever and provides information about the local surface potential by measuring the contact potential difference (CPD) between the sample and the AFM tip. This requires a transparent substrate with a back-gate on which markers can be generated using electron beam- or optical-lithography. The combination of optical and KPFM techniques allows the study of energy-band profiles and the generation of charge-carriers and their concentrations.

HL 13.53 Mon 15:00 Poster E

**Trench-etched In-Plane-Gate Transistors: Fabrication, Characterization, Logical Gates and Simulation** — •Lennart Anderson[1], Phil Badura[1], Matthias Kroll[2], Benjamin Feldern[1], Arne Ludwig[1], and Andreas Wieck[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Experimental Physics IV - Solid State Physics, Ruhr-Universität Bochum

In contrast to conventional field effects transistors (FETs), in which the channel is modulated by a perpendicular electric field, in the In-Plane-Gate transistor (IPGT) gate and channel (and hence source and drain) are in the same plane, leading to a lateral field effect and hence to a two-dimensional system.

In $GaAs/Al_xGa_{1-x}As$ high electron mobility structures conducting channels were defined in a two-stage wet chemical etching process. Current-voltage measurements show characteristic transistor behaviour. A NAND gate is realized based on a single IPGT, showing clear input-output characteristics. Interconnecting several NAND gates, all further basic logical gates, i.e. AND, OR, NOR, XOR and NOT, are realized. The IPGT structure is modelled in *nextnano++*, and its band structure is obtained by solving the self consistent Schrödinger-Poisson equation numerically. The effect of geometric parameters, i.e. trench width and channel width, as well as the applied gate voltages on the band structure and hence the transistor behaviour is studied. We find that surface states have a significant influence and provide a simple electrostatic model.

HL 13.54 Mon 15:00 Poster E

**Investigating Performance Limiting Recombination of Perovskite/C60 Interfaces using First Principle Calculations** — •Richard Gundermann[1], Felix Lang[1], Christopher Penschke[2], Peter Saalfrank[2], Filippo De Angelis[3], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Institute of Chemistry, University of Potsdam, Germany — [3]Department of Chemistry, Biology and Biotechnology, University of Perugia, Italy

Perovskite semiconductors became an interesting field to overcome the limitations of standard silicon based photovoltaic (PV) technologies. However, it is shown that performance-limitations are largely caused by significant nonradiative recombination at the perovskite/organic electron transport layer junctions. Especially the extensively used perovskite/$C_{60}$ junctions appear to have a reduction in PLQY within the first 1nm of $C_{60}$, which indicates nonradiative across-interface recombinations [1]. In this work, we investigate for the origin of these recombinations, e.g., packing faults in the first $C_{60}$ layer or inhomogeneous electrostatics. Also, electron-transfer-rates are discussed. Therefore, we use DFT calculations, including structure optimization of a perovskite/$C_{60}$ supercell. For reduced computational effort we also investigate for empirical Tight-Binding-Models to access heterostructure-modeling and features as transport properties.

[1] Warby, J. et al., Understanding Performance Limiting Interfacial Recombination in pin Perovskite Solar Cells. Adv. Energy Mater. 2022, 12, 2103567. https://doi.org/10.1002/aenm.202103567

HL 13.55 Mon 15:00 Poster E

**Characterization of Arsenic- and Antimony-Containing Layers Grown in a Source-Material Transformed MBE** — •Peter 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 Festkörperpysik, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany

The results of the growth of arsenic- and antimony-containing layers are presented. These layers were grown in a MBE system which underwent a transformation from II-VI (HgCdTe) to III-V (AlGaIn-AsSb) materials growth.

RHEED is utilized to determine surface reconstructions and growth rates *in situ*. Post-growth atomic force microscopy is employed to study the surface properties, such as roughness, step density and terrace width of the grown layers. With photoluminescence spectroscopy mapping of quantum well samples the radiative recombination yield on a whole wafer is compared between different samples. As a measure of epitaxial layer quality Hall-effect measurements on high electron mobility structures are performed.

These works represent the early steps after the commissioning of a used MBE system towards the growth of mid-IR emitters.

HL 13.56 Mon 15:00 Poster E

**Photoemission study and band alignment of GaN passivation layers on GaInP(100) heterointerfaces** — •Sahar Shekarabi[1], Mohammad Amin Zare Pour[1], Haoqing Su[2], Wentao Zhang[2], Chengxing He[2], Oleksandr Romanyuk[3], Agnieszka Paszuk[1], Shu Hu[2], and Thomas Hannappel[1] — [1]Grundlagen von Energiematerialien, Institut fur Physik, Technische Universit at Ilmenau, 98693 Ilmenau, Germany — [2]Department of Chemical and Environmental Engineering, Yale University, New Haven, CT 06520, USA — [3]FZU Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague 16200, Czech Republic

GaInP(100) is commonly used as a top photoabsorber in tandem devices and photoelectrochemical (PEC) cells. Since the photo corrosion degrades the cell stability and efficiency, GaN is used as a promising passivation layer. Therefore, studying the band alignment at this heterointerface is crucial for efficient charge transfer and minimizing photovoltage losses. Here, we study the band alignment of the multijunction heterostructure by X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy. GaInP(100) layers were grown by metalorganic chemical vapor deposition on top of GaAs(100), with a P-rich surface reconstruction. GaN passivation layers were grown by atomic layer deposition on oxidized GaInP(100) surfaces. On the P-rich n-GaInP(100) we found upward surface BB of 0.44 eV. Oxidation partly passivates surface states, lowering BB to 0.16 eV. Between the GaInP(100) and GaN passivation layer, we found a VBO of 1.9 eV, suggesting efficient electron transport but impeding hole transport.

HL 13.57 Mon 15:00 Poster E

**Comparison of multiple methods to determine the growth rate of MBE-grown layers** — •Timo A. Kurschat[1,2], Sascha R. Valentin[1], Peter Zajac[2], Arne Ludwig[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

This work compares multiple methods to determine the growth rate and thickness of thin layers grown by MBE.

The first method used is RHEED, which is the standard method to determine the growth rate in-situ. In contrast, the other measurements can only be carried out post-growth. One of these is photo-

luminescence (PL) spectroscopy. By measuring a sample containing multiple quantum wells and comparing it with the calculated emission energies, the widths of the quantum wells were calculated. Because our PL setup is capable of mapping entire wafers, deviations of the thickness can be seen. By stopping the rotation of the wafer during the growth of a quantum well, a thickness gradient is visible via an energy shift of the corresponding PL peak. The resulting growth rate can be used to derive the beam profile of the effusion cell. Three further methods make use of a sample with a distributed bragg reflector. Firstly, its reflectivity was measured and compared to simulations using the matrix-transfer method. Secondly, the thickness of the grown layers were measured using interference microscopy. Thirdly, AFM measurements were performed on the cleaved edge of the sample and the material contrast is utilized to obtain the layer thickness.

HL 13.58 Mon 15:00 Poster E

**Spherical harmonics expansion method for a semi-classical matrix transport equation describing spin dynamics in semiconductors** — •Felix Willert and Franz Xaver Bronold — Institut für Physik, Universität Greifswald, 17489 Greifswald, Germany

We discuss the transport of hot electrons, originating from a magnetized ferromagnet, in a semiconductor and the spin dynamics governed by the D'yakonov-Perel (DP) mechanism, which is the dominant spin relaxation process in semiconductors without inversion symmetry in the unit cell. For that we use a semi-classical model, where charge transport and scattering processes are described classically, but the spin-processes follow a quantum mechanical description. Due to the fact, that the DP mechanism changes the orientation of the spin and not directly its magnitude, it is not sufficient to describe the dynamics by two coupled equations for spin-up- and spin-down-electrons. Therefore we derive a Boltzmann equation for 2x2-density matrices in spin space with an additional term governing the DP process. To solve this equation, the H-Transformation and a spherical harmonics expansion is used.

Preliminary numerical results are presented, showing energy relaxation and partial thermal equilibration of the electron distribution as well as the spin relaxation throughout the system, which is strongly dependent on the energy, due to the DP mechanism depending on the third power of the electron momentum.

HL 13.59 Mon 15:00 Poster E

**Strongly driven germanium quantum dot** — •Bashab Dey and John Schliemann — University of Regensburg, Regensburg, Germany

Hole qubits in germanium quantum dots are promising candidates for coherent control and manipulation of the spin degree of freedom. The suppression of contact hyperfine interaction due to p-character of the holes, isotopic purification and absence of valley degeneracies are favourable for sustaining longer spin coherence and relaxation times in these systems. Furthermore, stronger spin-orbit interaction in germanium hole states facilitates faster qubit operations in these dots as compared to silicon or III-V semiconductors. Quantum NOT gates can be realized using these qubits through electric dipole spin resonance (EDSR) where Rabi oscillations are induced between the spin-up and -down states using ac-gate voltages. In this work, we theoretically study the time dynamics of a single hole qubit in a laser-driven planar germanium quantum dot confined laterally by a parabolic potential in presence of Rashba spin-orbit coupling(s) and a perpendicular magnetic field. We employ different methods such as Floquet theory and unitary transformations to study the time evolution of the qubit under the laser field. We obtain approximate analytical formula for the Rabi oscillations using a Schrieffer-Wolff transformation and establish a connection of our model with the ESDR results obtained for this system.

HL 13.60 Mon 15:00 Poster E

**Characterizing time resolved random laser and cavity exciton polariton supported random laser action in disordered ensembles of the hybrid perovskite CH3 NH 3 PbBr 3 (MAPB)** — •Regine Frank[1,2], Paul Bouteyre[3], Hai Son Nguyen[4,5], Christian Seassal[4,5], Emmanuelle Deleporte[3], and Bart A. van Tiggelen[6] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]Université Paris-Saclay, ENS Paris-Saclay, CNRS, CentraleSupélec, LuMIn, Gif-sur-Yvette, France — [4]Université de Lyon, Institut des Nanotechnologies de Lyon, INL/CNRS, Ecole Centrale de Lyon, Ecully, France — [5]Institut Universitaire de France (IUF), Paris, Franceb — [6]Universite Grenoble Alpes, Centre National de la Recherche Scientifique, LPMMC, Grenoble, France

We present semi analytical as well as numerical results (WENO) for photonic transport and Anderson localization of light in active disordered ensembles of the hybrid perovskite CH3 NH 3 PbBr 3 (MAPB) capped by PMMA. We compare experiments of two dimensional and three dimensional transport to time ans space resolved numerical results in the sense of finding the mechanism of coherent feedback for directed random laser emission and exciton-polariton supported random laser emission. This includes the analysis of the interplay of light-matter interaction in the sense of dynamics within the pumped microstructure with the mesoscopic physics of photonic transport in disordered and quasi ordered ensembles.

## HL 14: Poster II

Topics:
- Quantum dots and wires
- Quantum transport and quantum Hall effects
- Spin phenomena in semiconductors

Time: Monday 15:00–18:00 Location: Poster F

HL 14.1 Mon 15:00 Poster F

**Restoral of the Single-Photon Purity at a 2$\pi$ Excitation of a Quantum Two-Level System** — •Patricia Kallert[1], Lukas Hanschke[1], Melina Peter[2], Ailton José Garcia Junior[2], Eva Schöll[1], Saimon Filipe Covre Da Silva[2], Santanu Manna[2], Armando Rastelli[2], and Klaus D. Jöns[1] — [1]PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria

Exploring the properties of single-photons and their generation from for instance semiconductor quantum dots is critical to developing photonic quantum technologies. The coupling of resonant, coherent laser pulses to a quantum two-level system leads to Rabi rotations between the ground and excited state. In a dephasing-free system, a 2$\pi$ rotation then leads to either (i) two population inversions and therefore no photon emission or (ii) the emission of two successive photons, if after an emission during the presence of the pulse the system is re-excited.[1] Due to the different temporal shapes, the consecutive photons exhibit different spectral bandwidths, as related by the Fourier transform limit. Here we verify this prediction of different bandwidths for both photons using narrow filtering. By filtering the spectrally broad first photon, we*re reducing the probability of detecting two photons from the same excitation pulse. Our study should help to identify the optimal excitation conditions for applications in quantum technologies.

HL 14.2 Mon 15:00 Poster F

**Examination of charge carrier dynamics and their influence on mechanical curvature in a highly strained bent single AlxIn1-xAs/GaAs core shell nanowires as function of diameter via optical laser excitation and X-ray probe method** — •Taseer Anjum[1], Francisca Marín Largo[2], Philipp Jordt[3], Ali Al Hassan[5], Rajendra Prasad Giri[3], Lukas Petersdorf[3], Vahid Salehi[1], Matthias Rössele[4], Bridget Murphy[3], Oliver Brandt[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Ger-

many — [3]Institute of Experimental and Applied Physics, Kiel, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany — [5]Karlsruhe Institute of Technology, Karlsruhe, Germany

Extreme bending of semiconductor nanowires (NWs) through asymmetric shell deposition, creates strain gradients that impact their electronic properties. This deformation induces a gradient in the electronic band gap, fostering the formation of an intrinsic quasi-electric field. The study delves into understanding spatially complex electric fields via time-resolved nano x-ray diffraction experiments, tracking elastic deformation in bent NWs. Observation of the GaAs NW 111 Bragg peak evolution reveals plastic deformation due to excess photoexcited charge carriers, mitigated by laser fluence adjustment. This exploration leads to the direct observation of eigenmodes associated with piezo-flexoelectric field screening in bent NWs.

HL 14.3 Mon 15:00 Poster F

**Microscopic Simulations of Photonic Cluster-State Generation with Lambda-Type Systems** — •Nikolas Köcher, David Bauch, Nils Heinisch, and Stefan Schumacher — Physics Department, CeOPP, and PhoQS, Paderborn University, Germany

In this work, we conduct an in-depth exploration of microscopic quantum-mechanical simulations of the deterministic generation of photonic cluster states from lambda-type systems, with a particular focus on time-bin encoded linear cluster states. Our analysis includes a thorough examination of second and third order time-bin correlations, including stabilizer generator expectation values to quantify the quality of the generated states. The foundation of our exploration lies in the lambda-type system, where proposed protocols for deterministic generation are established [1], utilizing a hole-spin qubit in quantum dot molecules. The quantum dot molecule's lambda system serves as the backdrop for our simulations, providing detailed insights into the efficiency and viability of the proposed protocols. Our aim is to contribute to the understanding of these quantum systems and their potential applications in the generation of highly entangled photonic cluster states [2], considering both the quality and localizable entanglement in the generated quantum states. [1] Vezvaee et al., Phys. Rev. Appl. 18.L061003 (2022). [2] Raissi et al., arXiv preprint 2211.13242 (2022).

HL 14.4 Mon 15:00 Poster F

**Acoustic control of light scattering from a single-photon emitter in the strong driving limit** — •Daniel Wigger[1] and Paweł Machnikowski[2] — [1]Fachbereich Physik, Universität Münster, Münster, Germany — [2]Institute of Theoretical Physics, Wrocław University of Science and Technology, Wrocław, Poland

In the recent developments of quantum technologies, the combination of different solid state excitations into hybrid infrastructures renders a promising perspective to circumvent drawbacks of individual approaches. In this context phonons represent a versatile platform to dynamically manipulate charge carriers or spin degrees of freedom in the solid state [1]. We have recently demonstrated that in the weak optical driving limit the single-photon emission characteristics of quantum dots can be precisely controlled by surface acoustic waves (SAWs) in the spectral and the temporal domain [2]. We have also made the first steps towards acousto-optical quantum transduction [3].
In this contribution we discuss the opportunities of SAW control of spectral tuning of single emitter spectra in the strong driving limit where the spectrum is given by the Mollow triplet. We find theoretically that phonon sidebands develop which involved mixing behaviors that can exhibit crossing, anticrossing, and extinction behaviour.
[1] Adv. Quantum Technol. 4, 2000128 (2021); IEEE Trans. Quantum Eng. 3, 5100217 (2022)
[2] Optica 8, 291 – 300 (2021); Phys. Rev. Res. 3, 033197 (2021)
[3] AVS Quantum Sci. 4, 011403 (2022); Adv. Quantum Technol. 2300153 (2023)

HL 14.5 Mon 15:00 Poster F

**Assessing the alignment accuracy of state-of-the-art deterministic fabrication methods for single quantum dot devices** — Abdulmalik Madigawa[1], •Jan Donges[2], Benedek Gaal[1], Shulun Li[2,3,4], Hanqing Liu[3,4], Deyan Dai[3,4], Xiangbin Su[3,4], Xiangjun Shang[3,4], Haiqiao Ni[3,4], Johannes Schall[2], Sven Rodt[2], Zhichuan Niu[3,4], Niels Gregersen[1], Stephan Reitzenstein[2], and Battulga Munkhbat[1] — [1]TU Denmark — [2]TU Berlin — [3]Institute of Semiconductors Beijing — [4]University of Chinese Academy of Sciences Beijing

The realization of efficient quantum light sources relies on the integration of self-assembled quantum dots (QDs) into photonic nanostructures with high spatial positioning accuracy. In this work, we present a comprehensive investigation of the QD position accuracy, obtained using two markerbased QD positioning techniques, photoluminescence (PL) and cathodoluminescence (CL) imaging, as well as using a marker-free in-situ electron beam lithography (in-situ EBL) technique. We employ four PL imaging configurations with three different image processing approaches and compare them with CL imaging. We fabricate circular mesa structures based on the obtained QD coordinates from both PL and CL image processing to evaluate the final positioning accuracy. We discuss the possible causes of the observed offsets, which are significantly larger than the QD localization uncertainty obtained from simply imaging the QD light emission from an unstructured wafer.

HL 14.6 Mon 15:00 Poster F

**A Versatile Transfer Printing Toolbox for Device Stacking** — •Ioannis Caltzidis[1], Oscar Camacho Ibarra[1], Normen Auler[2], Jan G. Hartel[1], Dirk Reuter[2], and Klaus D. Jöns[1] — [1]PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn — [2]Nanostructuring, Nanoanalysis and Photonic Materials, Department of Physics Paderborn University, Germany

To scale up photonic quantum technologies such as quantum communication, or quantum computing, integration in photonic circuits is required. One challenge is the efficient integration of single-photon emitters into photonic integrated circuits (PIC). The integration approaches of single photon emitters can be categorised into monolithic, heterogeneous and hybrid methods. Monolithic integration is the fastest in terms of fabrication overhead, while heterogeneous, and especially hybrid integration offers a diverse choice of materials and properties to be combined. Here we use molecular beam epitaxy-grown InxGa1-xAs/GaAs quantum dots integrated into a nanobeam cavity. The resulting nanophotonic device is transferred via a pick-and-place technique into a Lithium niobate on insulator (LNOI) waveguides which we fabricate using a triple-layer nanofabrication approach. We employ a thermal release transfer method with polypropylene carbonate as a release agent. The transfer stage's translational, rotational, and azimuthal degrees of freedom enable deterministic positioning and control in the fabrication process.

HL 14.7 Mon 15:00 Poster F

**Spectroscopic characterization of site-controlled quantum dots in hexagonal pillar arrays** — •Priyabrata Mudi, Martin Podhorský, Maximilian Klonz, Imad Limame, Kartik Gaur, Sven Rodt, and Stephan Reitzenstein — Institute for Solid State Physics, Technical University of Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

The integration of quantum dots (QDs) into nanoscale structures holds significant promise for advancing the fields of quantum information processing and optoelectronics. This study investigates site-controlled quantum dots embedded in hexagonal pillar arrays, offering precise positioning for applications in fiber coupling. Advanced spectroscopy explores optical properties, exciton dynamics and single photon emission characteristics of these nanostructures, guiding future quantum device design. The work examines growth parameters' influence on QD uniformity, establishing guidelines for fabrication precision. Controllable QD placement via the buried stressor concept is crucial for achieving reproducible and reliable quantum systems. The gained knowledge informs design principles for quantum systems, with implications for computing, secure communication, and optoelectronic devices.

HL 14.8 Mon 15:00 Poster F

**Quantum-state tomography of polarization-entangled telecom photons from semiconductor quantum dots** — •Ilenia Neureuther[1], Tim Strobel[1], Stefan Kazmaier[1], Tobias Bauer[2], Marlon Schäfer[2], Ankita Choudhary[3], Nand Lal Sharma[3], Raphael Joos[1], Cornelius Nawrath[1], Weijie Nie[3], Ghata Bhayani[3], André Bisquerra[1], Caspar Hopfmann[3], Simone L. Portalupi[1], Christoph Becher[2], and Peter Michler[1] — [1]Institut für Halbleiter und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology ($IQ^{ST}$) and SCoPE, University of Stuttgart, Allmandring 3, 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

For the future development of quantum communication, triggered

entangled-photon pairs are of fundamental importance. The integration of single photons into existing optical fiber networks requires the use of telecom wavelengths. Semiconductor quantum dots (QDs) are promising candidates for providing on-demand, indistinguishable polarization-entangled photon pairs. Here, we generate photons emitted via the biexciton-exciton cascade in GaAs QDs formed via Al droplet etching, emitting at 780nm. In a bi-directional polarization-conserving quantum frequency converter, we convert the biexciton emission to 1515nm. Polarization-entanglement is measured after the transmission through a 35km inner-city fiber network.

HL 14.9 Mon 15:00 Poster F

**Investigation of Temperature Dependent Intensity Anomalies of Local Droplet Etched Gallium-Arsenide Quantum Dots** — •Sayed Shkeebullah Sadat, Hans-Georg Babin, Andreas Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Bochum, Deutschland

Liquid droplet etched (LDE) quantum dots (QD) made with molecular beam epitaxy (MBE) show an interesting behavior when photoluminescence (PL) spectroscopy is performed: during the growth process of the QDs an AlAs-wall can emerge around the nanoholes, which acts as a potential barrier between the QDs and the surrounding wetting layer (WL). By temperature- and power-dependent measurements anomalous behavior of photoluminescence intensity can be observed * in the here measured range of 83K-283K the intensity increases significantly to a certain sweetspot-temperature, before decreasing due to thermally activated non-radiative recombination. This initial behavior can be explained by an increase of available charged carriers from the WL with increasing temperature. Here not only the generation and recombination of excitons play an important role, but specifically the influence of temperature on thermally activated and assisted processes such as overcoming the barrier between WL and QDs and tunneling through the barrier. As part of this work a rate equation is developed, which considers the different thermal dependencies and thus should provide a quantitative insight into the complex anomalous behavior.

HL 14.10 Mon 15:00 Poster F

**Growth Optimization and fabrication of Site-Controlled InGaAs Quantum Dots in Hexagonal Arrays** — •Martin Podhorský, Imad Limame, Kartik Gaur, Maximilian Klonz, Priyabrata Mudi, Sven Rodt, and Stephan Reitzenstein — Institute of Solid State Physics, Technical University of Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Optimized site-controlled quantum dots (SCQD) arrays have significant potential for practical applications in fields such as quantum computing and secure communication. This study focuses on the growth and optimization of InGaAs SCQDs within hexagonal arrays, aiming to enhance the precision and reliability of the quantum dot placement for advanced optoelectronic applications. We employ a systematic approach to optimize growth parameters to achieve uniform and reproducible site-controlled growth. The impact of these growth conditions on the structural and optical properties of SCQDs is thoroughly investigated via atomic force microscopy (AFM), scanning electron microscopy (SEM), confocal laser scanning microscopy (CLSM), X-Ray diffraction (XRD) and photoluminescence (PL) spectroscopy.

HL 14.11 Mon 15:00 Poster F

**Hybrid combination of InGaAs-QDs and Si-based photonic integrated circuits for telecom wavelengths** — •Elias Herzog[1], Ulrich Pfister[1], Daniel Wendland[2], Ponraj Vijayan[1], Lena Engel[1], Peter Gierss[1], Erik Jung[3], Michael Jetter[1], Simone L. Portalupi[1], Wolfram Pernice[2,3], 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, Germany — [2]Physikalisches Institut AG Pernice, University of Münster, Heisenbergstraße 11, Germany — [3]Kirchhoff-Institut für Festkörperforschung, University of Heidelberg, Im Neuenheimer Feld 227, Germany

Silicon based materials are widely used for photonic integrated circuits (PICs), because of their low losses in the telecom wavelength regime and available manufacturing expertise. These properties makes them suitable for potential large scale PICs for on-chip quantum technologies. On demand single-photon sources are hard to realize in these systems, due to the indirect bandgap of silicon. On the other hand, InGaAs Quantum Dots (QDs) can emit high quality single photons at telecom wavelengths making it desirable to combine both material platforms. Here we discuss our first steps in combining the benefits of III-V QDs and SiN photonic chips.

HL 14.12 Mon 15:00 Poster F

**A model study on multiple optically driven emitters coupled to a common phononic environment** — •Daniel Groll[1], Daniel Wigger[2], and Tilmann Kuhn[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany

Single photon emitters in a solid state environment are inevitably coupled to the phonon modes of the host material. While this interaction channel is often seen as a drawback, leading to decoherence, it also allows for control of emitters via phonons in the context of hybrid quantum systems. Here we investigate the optically induced dynamics of multiple emitters interacting with a common phononic environment and show that such a coupling leads to an effective interaction between the spatially separated emitters.

In the case of emitters coupling strongly to a single phonon mode, e.g., realized by multiple quantum dots embedded in a surface acoustic wave resonator, we predict distinct deviations from the Mollow triplet spectrum in resonance fluorescence under strong optical driving.

In the case of coupling to an anharmonic phonon bath, leading to pure dephasing in addition to the effective emitter-emitter–coupling, we investigate the complex dynamics of such a driven-dissipative quantum system.

HL 14.13 Mon 15:00 Poster F

**Self-assembly based quasi-1D metallic nanowires** — Borja Rodriguez-Barea[1], •Raghda Abdelfattah[1], Charlotte Kielar[1], Ulrich Kemper[2], Jingjing Ye[2], Foram Joshi[3], Brenda Romero-Palestino[3], Ralf Seidel[2], Stefan Diez[3], and Artur Erbe[1] — [1]Institute of Ion Beam Physics und Material Science, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany — [3]B CUBE - Center for MolecularBioengineering, TU Dresden, Germany

Self-assembly, autonomous organization of materials into hierarchical structures, offers a unique bottom-up approach for the controlled fabrication of electronic components. Potentially, self-assembled low-dimensional materials could be integrated into functional architectures without the need of expensive cleanroom tools and facilities.

Here we report a study on the electrical characterization of quasi-1D metallic nanostructures using two biotemplates. The first employs the DNA origami technique, while the second utilizes the microtubule lumen for growth. In both cases, metallic seed nanoparticles are bound to the template and reduced forming a continuous nanowire. Thus, the shape and length of the wire can be controlled. The electrical characterization data shows two kinds of transport behaviours: linear and non-linear current-versus-voltage responses, depending on the continuity of the metal nanowires. Temperature-dependent charge transport measurements reveal the dominating mechanisms along these wires, offering an insight into the reliability for this cost-effective electronic device fabrication.

HL 14.14 Mon 15:00 Poster F

**Thermal scanning probe lithography (t-SPL) for quasi-1D DNA origami-based Pd nanowires** — •Raghda Abdelfattah[1], Borja Rodriguez-Barea[1], Charlotte Kielar[1], Ulrich Kemper[2], Jingjing Ye[2], Ralf Seidel[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics und Material Science, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

Theoretically, low-dimensional materials are sensitive and damaged by high energetic e-beams reducing the device conductance. Non-invasive thermal scanning probe lithography (t-SPL) has lead to clean and undamaged contact areas to atomically thin materials after pattering, reporting lower contact resistance from patterned electrodes.

In this work, we have turned our eyes to studying the recently reported DNA origami-based Pd nanowires and further performing electrical characterization to reveal the charge transport mechanism in such kind of structures. We aim to use thermal probe lithography, specifically the Nanofrazor, as a top-down fabrication tool to pattern multiple electrodes positioned on top of such nanowires. The main advantage of this technique is given by the fact that imaging of the nanostructures can be performed at the same time as structuring the electrodes. This increases the precision of contacting without the requirement of additional alignment markers. Hence, it allows us to perform electrical local characterization through various segments of the

wire, providing an insight into the relationship between the nanowires' morphology and its electronic properties.

HL 14.15 Mon 15:00 Poster F

**Two-color resonant excitation to study the Auger effect in a single photon emitter** — •Nico Schwarz[1], F. Rimek[1], H. Mannel[1], M. Zöllner[1], B. Maib[1], A. Ludwig[2], A. D. Wieck[2], A. Lorke[1], 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 quantum dot (QD) as a single photon emitter is an ideal system to study the Auger effect in a confined nanostructure. The recombination energy is transferred to a third charge carrier that leaves the dot [1], hence, the Auger effect destroys the radiative recombination of the negatively charged exciton (trion $X^-$) - an effect, which should be minimized in future optical applications. In order to minimise the Auger recombination, we studied the effect of an applied magnetic field on the Auger recombination [2]. However, in a magnetic field, the trion transition of the QD is no longer spin degenerate, and besides the Auger recombination, the spin-flip and spin-flip Raman transitions make it difficult to determine the Auger rate. Here, we use two-color time-resolved resonance fluorescence measurements with two-color spectral analysis of the emitted single photons from the QD to distinguish between the different state transitions. In this way, spin relaxation and spin-flip Raman scattering can be neglected. This ensures that we can directly measure all important transition and tunneling rates into the quantum dot and get a high accuracy for the influence of the magnetic field on the Auger rate. [1] P. Lochner et al., Nano Lett. **20**, 1631-1636 (2020). [2] H. Mannel et al., JAP **134**, 154304 (2023).

HL 14.16 Mon 15:00 Poster F

**Towards Low Temperature Imaging of Telecom Wavelength InGaAs Quantum Dots** — •Lukas Wagner, Stephanie Bauer, Ponraj Vijayan, Michael Jetter, Simone Luca Portalupi, 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

Semiconductor quantum dots are a promising non-classical light source for quantum information technology. To boost the fabrication yield of bright single and entangled photon pair sources, deterministic fabrication techniques can be employed. For this purpose, three techniques have been developed: low temperature deterministic optical lithography, low temperature deterministic electron beam lithography, and low temperature imaging, with recent interesting results also at telecommunication wavelengths. Markers from electron-beam lithography are used as reference points for determining the position of viable quantum dots for deterministic fabrication of spatially and spectrally matching micro cavities. Using standard micro photoluminescence techniques at telecom wavelengths for preselection and precise position determination is effective, but there is room for improvement in the upscaling of the process. To tackle this challenge an imaging setup is employed to speed up and enhance the precision of determining the position. In this contribution, a precise comparison between low temperature lithography and low temperature imaging at telecommunication wavelength will be discussed.

HL 14.17 Mon 15:00 Poster F

**Deterministically fabricated InAs/InP quantum dot-based single-photon sources at telecom wavelengths** — •Monica Pengerla[1], Yury Berdnikov[2,3], Pawel Holewa[2,3], Alexander Kosarev[1], Sven Rodt[1], Elizaveta Semenova[2,3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [2]DTU Electro, Technical University of Denmark, Kongens Lyngby, Denmark — [3]NanoPhoton-Center for Nanophotonics, Technical University of Denmark, Kongens Lyngby, Denmark

Quantum dot (QD) based single-photon sources are key elements of photonic quantum networks. In huge demand are sources emitting at telecom wavelengths, especially in the C-band at 1.55 $\mu$m, which enables long-distance fiber-based quantum communication. Here, we report the development of single-photon sources based on InAs/InP QDs in circular Bragg grating photonic cavities with back-side Al mirror and bonded to the Si substrate. Numerical simulations of such quantum devices reveal a noticeable rise of photon extraction efficiency beyond 80% for NA = 0.65, as well as Purcell enhancement of the QD transition rate. The devices are deterministically fabricated using a state-of-the-art electron beam lithography system with integrated cathodoluminescence (CL) at 20 K, allowing us to perform in situ electron beam lithography with a high spectral and spatial resolution. Micro-photoluminescence studies reveal cavity-enhanced emission and excellent quantum optical properties from the deterministically fabricated quantum devices.

HL 14.18 Mon 15:00 Poster F

**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 can form a spin qubit with the singlet ground state. It is electrically adressable and therefore of interest for quantum information processing. This requires a long coherence time $T_2$, which is limited by the spin relaxation time $T_1$. While $T_1$ has already been investigated by optical measurments, we present our all-electrical measurment approach.
We embedded a layer of InAs/GaAs QDs in an inverted high electron mobility transistor (HEMT) to selectively charge and discharge the QD states with electrons from a tunnel-coupled electron reservoir (2DEG). The 2DEG acts as a sensitive detector for the charge in the QD layer. By using time-resolved transconductance spectroscopy [1] and altering the charging times we can observe the relaxation from the triplet excited state to the singlet ground state. We extract the relaxation time $T_1$ by applying a rate equation model. While there are already first results for $T_1$ [2], ongoing questions of interest are its dependency of the strength and orientation of an external magnetic field.
[1] B. Marquardt. et al., Nature Commun. 2, 209 (2011)
[2] K. Eltrudis. et al., Appl. Phys. Lett. 111, 092103 (2017)

HL 14.19 Mon 15:00 Poster F

**Investigation of the correlation of optical and electronic properties of O-band quantum dots** — •Danial Kohminaei, Nikolai Spitzer, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum; Lehrstuhl für angewandte Festkörperphysik, Bochum, Deutschland

For future applications in telecommunications and information technology, quantum dots (QDs) are promising candidates as single photon sources. Optical signals are transmitted over long distances through optical fibers, within which the light is attenuated by Rayleigh scattering and by infrared absorption. However, at the so-called Telecom O-band at 1310nm there is a local minimum of absorption.

We grow self-assembled InAs QDs in InGaAs quantum wells via molecular beam epitaxy; understanding the correlation between growth parameters and the resulting structure defining the optical and electronic properties of the QDs is topic of cutting-edge research.

Therefore, the distribution and properties of QDs on a sample with a pattern defining layer (PDL) [1] underneath the QDs and a InGaAs strain reduction layer above are measured by photoluminescence (PL) and capacitance-voltage C(V) spectroscopy mapping.

[1] BART, N. et al.: Wafer-scale epitaxial modulation of quantum dot density, Nature Communications 13 (2022)

HL 14.20 Mon 15:00 Poster F

**Circular gratings for efficient light extraction from InAs quantum dots** — •Frederik Ernst[1], Stefan Linden[1], Paul Steinmann[1], and Beata Kardynal[2] — [1]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany — [2]PGI-9, Forschungszentrum Jülich, Jülich, Germany

Indium arsenide quantum dots are recognized as high-quality single photon sources. Since the quantum dots are however, embedded in a high refractive index material (GaAs), efficient outcoupling of the photons is challenging. In order to increase the efficiency of light extraction from the GaAs host, we investigate circular gratings (bullseye structure) made from tantalum pentoxide that are positioned on the GaAs surface above individual quantum dots. Our approach involves optimizing the design of these bullseye structures through numerical calculations based on the Finite-Difference-Time-Domain (FDTD) method. The production of these structures, targeted at selected quantum dots, is achieved using electron beam lithography with a positive-tone resist, followed by electron beam evaporation to deposit a 70 nm thick tantalum pentoxide film. Optical experiments conducted at liquid helium temperatures (T=4 K) include exciting the quantum dots with a 785 nm wavelength laser and recording their PL emission before and after

bullseye deposition. Preliminary analysis suggests an enhancement in light extraction efficiency, indicating promising applications in quantum dot technologies for improved photonics systems. Ongoing analysis aims to quantify this increase, potentially offering a significant advancement in photon manipulation at the quantum level.

HL 14.21 Mon 15:00 Poster F

**Oscillator strength of quantum dots from ensemble photoluminescence** — •Yannis Rüggen, Nikolai Spitzer, Arne Ludwig, and Andreas D. Wieck — Ruhr-Universität Bochum; Lehrstuhl für Angewandte Festkörperphysik, Bochum, Germany

A special type of semiconductor heterostructures are so-called quantum dots, which have a potential confinement in all spatial dimensions and therefore have discrete energy levels.

In this project, self-organized InAs quantum dots grown by molecular beam epitaxy are investigated. These quantum dots are In-flushed and gradient-grown and will be examined via power-dependent photoluminescence spectroscopy. Based on the laser power, the lifetime of the excitons will be estimated relatively. Two assumptions are made for this. Firstly, it is assumed that there is a direct correlation between the intensity and the quantum dot density. Furthermore, it is assumed that the lifetime is constant over the entire wafer. The aim of the project is to develop a simple method for estimating the lifetime of excitons. Subsequently, this will be verified by lifetime measurements.

HL 14.22 Mon 15:00 Poster F

**Telecom wavelength InP based quantum dots: Growth and optical characterization** — •Ranbir Kaur, Mohanad Alkaales, Johann Peter Reithmaier, and Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Germany

Due to their atomic-like properties such as a size-dependent bandgap and strong quantum confinement, semiconductor quantum dots (QDs) emitting at the telecom wavelengths are promising candidates for quantum communication. InP-based QD material system is one of the possible candidates to achieve this spectral region due to the low lattice mismatch (3.2%) between InP and InAs. [1, 2].

Here, we report molecular beam epitaxy growth optimization of InAs/InP QDs emitting at telecom wavelengths for quantum communication applications. Photoluminescence (PL) and Atomic force microscopy (AFM) were used to study the effects of growth parameters on optical and morphological properties. QDs were grown on high-quality distributed Bragg reflectors (DBRs) with 99% reflectivity and lattice-matched lattices to enhance extraction efficiency. Micro-PL measurements at low temperatures reveal bright single QD emission around 1.55 micrometer with narrow linewidths and small fine-structure splittings. Moreover, we report on the growth and optical analysis of C-band QD molecules.

[1] Benyoucef et al., Appl. Phys. Lett. 103 162101 (2013)
[2] Kors et al., Appl. Phys. Lett. 112, 172102 (2018)

HL 14.23 Mon 15:00 Poster F

**Design of a Majorana trijunction** — •Juan Torres[1], Sathish Kuppuswamy[2], and Anton Akhmerov[2] — [1]QuTech, Delft, The Netherlands — [2]Kavli Institute of Nanoscience, Delft, The Netherlands

Braiding of Majorana states demonstrates their non-Abelian exchange statistics. One implementation of braiding requires control of the pairwise couplings between all Majorana states in a trijunction device. To have adiabaticity, a trijunction device requires the desired pair coupling to be sufficiently large and the undesired couplings to vanish. In this work, we design and simulate a trijunction device in a two-dimensional electron gas with a focus on the normal region that connects three Majorana states. We use an optimisation approach to find the operational regime of the device in a multi-dimensional voltage space. Using the optimization results, we simulate a braiding experiment by adiabatically coupling different pairs of Majorana states without closing the topological gap. We then evaluate the feasibility of braiding in a trijunction device for different shapes and disorder strengths.

HL 14.24 Mon 15:00 Poster F

**Current Induced Magnetization Switching in Vanadium doped $(Bi_xSb_{1-x})_2Te_3$** — •Boris Stanchev, Daniel Rosenbach, Gertjan Lippertz, Anjana Uday, Alexey Taskin, Yoichi Ando, and Erwann Bocquillon — Universität zu Köln, II. Physikalisches Institut, Zülpicher Str. 77, Cologne, Germany

Thin-film quantum anomalous Hall (QAH) insulators host chiral one dimensional edge states when magnetized at mK scale temperatures. The chirality of these edge states corresponds with the direction of the magnetization. Recent experiments have shown that the chirality of edge states and magnetization direction in QAH insulators can also be switched by applying a large current beyond the breakdown threshold at which the QAH effect degrades. However, the precise mechanisms and conditions that lead to this current switching have yet to be elucidated. Thus we present progress towards further studies where we also replicate this effect in Vanadium doped $(Bi_xSb_{1-x})_2Te_3$. Possible applications include the study of ferromagnetic domain walls in QAH insulators, and in particular the coupling of co-propagating edge channels.

HL 14.25 Mon 15:00 Poster F

**Real-Space Renormalisation Group Approach to the Quantum Spin-Hall Effect** — Syl Shaw and •Rudolf Roemer — University of Warwick, Coventry, United Kingdom, CV4 7AL

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. In our work, we extend a previously developed real-space renormalisation group (RSRG) method to study the time-reversal invariant Chalker-Coddington model. The value of the critical exponent of the localisation length in the quantum Hall situation is at present accepted to be $\nu = 2.59 \pm 0.01$. Previous work based on the RSRG approach gives a much lower $\nu = 2.39 \pm 0.01$. We now increase statistics and the accuracy of each RG step to improve the RSRG-based estimate. We find an increased value of $\nu = 2.55 \pm 0.02$. We then generalise the RSRG method to the time-reversal case and determine $\nu$ in this symmetry class.

HL 14.26 Mon 15:00 Poster F

**Investigation of quantum anomalous Hall edge states using thermal noise measurements** — •Alina Rupp, Daniel Rosenbach, Boris Stanchev, Anjana Uday, Gertjan Lippertz, Alexey Taskin, Yoichi Ando, and Erwann Bocquillon — Physics Institute II, University of Cologne, Cologne, Germany

In 3D topological insulators (TIs) transport is governed by 2D topologically protected surface states. By magnetically doping the TI quantum anomalous Hall insulators can be created which exhibit a single chiral edge state and a quantized Hall conductance. Besides the electronic transport, heat transport is also quantized. We aim to observe this using thermal noise measurements.

As a basis for our experiment, we use thin films of V-doped $(Bi_xSb_{1-x})_2Te_3$ grown by molecular beam epitaxy which are etched into a bow tie shape. In the center of the bow tie, we define a metallic island that is heated via the Joule effect through one edge channel while through another edge channel the heat is evacuated. Due to the conductance quantization the Joule power heating the island is well defined, while the quantization of heat transport controls the rate at which this power is evacuated from the island. Thus, by measuring the temperature of the island using thermal noise, insights on the characteristics of the edge states can be gained. In order to detect small changes in the temperature we combine an LC resonator with low-noise amplifiers to enhance the measured signal. This setup has to be calibrated in terms of the amplification chain and the electron temperature to then be able to detect quantized heat transport.

HL 14.27 Mon 15:00 Poster F

**A study of Magnetic Topological Insulator $MnSb_2Te_4$ using the *GW* method** — •Mohammad Farhan Tanzim and Irene Aguilera Bonet — Science Park 904, 1098 XH Amsterdam

We present *GW* calculations of the magnetic topological insulator $MnSb_2Te_4$ within the all-electron full-potential linearized augmented-plane-wave formalism. Magnetic topological insulators are materials with a narrow band gap, which is often inaccurately predicted by standard Density Functional Theory (DFT) calculations and hence, the comparison with experimental band structures is often unsatisfactory. For this reason a perturbative correction to the Kohn-Sham eigenvalues and eigenstates is necessary. We do this via many-body perturbation theory in the *GW* approximation. Our *GW* calculations show that the band gap of these materials are comparable to the experimental data. However, we do not observe the topological surface states that are characteristic of magnetic topological insulators. For this reason, we are focusing our efforts on the accurate implementation of *GW*

calculations including both spin-orbit coupling (SOC) and magnetism. Previously, the SOC was added only as an a posteriori correction. This could be one of the reasons for not obtaining the correct orbital character of the valence and the conduction bands, which might lead to the wrong topological character and thus, account for the missing surface states. We also present progress done in that front so far.

HL 14.28 Mon 15:00 Poster F

**Nonlinear Spin to Charge Conversion and Thermopower in an inverted GaAs/AlGaAs 2DEG** — •Benedikt Gruenewald, Dieter Schuh, Dominique Bougeard, Dieter Weiss, and Mariusz Ciorga — Universität Regensburg, Regensburg, Germany

Generating and detecting a nonzero spin accumulation in nonmagnetic materials by electrical means is at the heart of spintronics. A typical electrical detection scheme of injected spins involves Silsbee-Johnson spin-charge coupling, where spin accumulation at the ferromagnet-nonmagnet interface is converted into the electromotive-force, linear in the spin accumulation, measured across the junction. In nanoscale devices, an alternative solution was proposed. It was shown, that energy-dependent transmission in quantum point contacts (QPC), narrow constrictions in a two-dimensional electron gas (2DEG), leads to the voltage measured across QPC being quadratic in the spin accumulation. Here we present the results of our experiments on employing a QPC as a nonlinear detector of spin accumulation generated electrically in a 2DEG formed in the inverted GaAs/AlGaAs heterojunction. We employ a Spin Esaki Diode to electrically inject spins from the ferromagnetic semiconductor (Ga,Mn)As into the 2DEG. Both local and nonlocal measurement techniques were employed. However, separating the contribution between spin and thermopower remains a challenge.

## HL 15: Quantum Dots and Quantum Wires (joint session TT/HL)

Time: Monday 16:45–18:15 Location: H 3007

HL 15.1 Mon 16:45 H 3007

**Quantum Dot Source-Drain Transport Response at Microwave Frequencies** — •Harald Havir — Lund University

Quantum dots are frequently used as charge sensitive devices in low temperature experiments to probe electric charge in mesoscopic conductors where the current running through the quantum dot is modulated by the nearby charge environment. Recent experiments have been operating these detectors using reflectometry measurements up to GHz frequencies rather than probing the low frequency current through the dot. In this talk I will present the work "Quantum Dot Source-Drain Transport Response at Microwave Frequencies" where we use an on-chip coplanar waveguide resonator to measure the source-drain transport response of two quantum dots at a frequency of 6 GHz with the aim to further increase the bandwidth limit for charge detection. Similar to the low frequency domain, the response is here predominantly dissipative. For large tunnel coupling, the response is still governed by the low frequency conductance, in line with Landauer-Büttiker theory. For smaller couplings, our devices showcase two regimes where the high frequency response deviates from the low frequency limit and Landauer-Büttiker theory: When the photon energy exceeds the quantum dot resonance linewidth, degeneracy dependent plateaus emerge. These are reproduced by sequential tunneling calculations. In the other case with large asymmetry in the tunnel couplings, the high frequency response is two orders of magnitude larger than the low frequency conductance G, favoring the high frequency readout.

HL 15.2 Mon 17:00 H 3007

**Relaxation to persistent currents in a Hubbard trimer coupled to fermionic baths** — •Nikodem Szpak[1], Gernot Schaller[2], Ralf Schützhold[2,3], and Jürgen König[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider a ring of fermionic quantum sites, modeled by the Fermi-Hubbard Hamiltonian, in which electrons can move and interact strongly via the Coulomb repulsion. The system is coupled to fermionic cold baths which by the exchange of particles and energy induce relaxation in the system. We describe the system effectively by the Lindblad master equations in various versions valid for different coupling parameter regimes. The early relaxation phase proceeds in a universal way, irrespective of the relative couplings and approximations. The system settles down to its low-energy sector and is consecutively well approximated by the Heisenberg model. In the late relaxation, different Lindblad approaches push the system towards different final states with opposite spin orders, from ferromagenetic to antiferromagnetic. Due to spin frustration in the trimer, degenerate ground states are formed by spin waves (magnons). The system described by the global coherent version of the Lindblad operators relaxes towards the final states carrying directed persistent spin currents.

[1] N. Szpak et. al., arXiv:2311.06331

HL 15.3 Mon 17:15 H 3007

**Spatially-resolved dissipation in a quantum wire with a coherent scatterer** — •Nico Leumer[1,2], Denis Basko[3], Rodolfo Jalabert[1], Dietmar Weinmann[1], and Robert Whitney[3] — [1]IPCMS, France — [2]DIPC, Spain — [3]LPMMC, France

The recent advent of astonishing measurement techniques allows the near-atomic resolution of tiny local temperature changes, even three orders of magnitude lower than the sample temperature itself [1]. The new approaches confirmed earlier estimations that dissipation (accompanying electric current) is not shared equally among two 1d wires attached to a point contact. Moreover, the formation of so called heat-spots (small and confined areas of increased temperature) were observed in the quantum regime [2]. Evidently, dc charge transport possesses the key to further unravel the microscopic mechanisms behind spatial dissipation profiles.

Based on a model of two 1d wires sandwiching a scatterer, we investigated the spatial distribution of the dissipated power for generic transmission of the scatterer. We present the mechanism behind the formation of heat/ cold spots and the key role of the electric potential, which is required to maintain the electric current against the increased wire's resistivity in close vicinity to the point contact. Additionally, we report on the self-consistent calculation of the steady state current which obeys a four-point Landauer type relation w.r.t. the voltage drop inside the scatterer.

[1] D. Halbertal et al., Nature 539 (2016) 407
[2] Q. Weng et al., Nat. Commun. 12 (2021) 4752

HL 15.4 Mon 17:30 H 3007

**Multi-terminal interacting-quantum-dot-based devices** — •Peter Zalom — Institute of Physics, Czech Academy of Sciences, Na Slovance 2, CZ-18200 Praha 8, Czech Republic

Recent breakthroughs in experimental physics pave the way for the creation of intricate nanoscale devices featuring three or more superconducting electrodes. Such multi-terminal systems differ markedly from conventional two-lead Josephson junctions due to the supercurrent distribution into the constituent terminals. Exerting full phase-control leads then to a multitude of practical applications.

In this talk, we explore the potential for using nanowires or carbon nanotubes in the central scattering region to enhance the existing functionalities via the underlying quantum phase transitions. Our findings, as elucidated in [1], lay the foundation for purely phase-controlled superconducting transistor and diode effects in three-terminal systems even in the absence of inter-lead couplings. Proceeding with more complex architectures requires, however, development of new Numerical Renormalization Group (NRG) methods to accommodate arbitrary gapped tunneling densities of states. This critical development, recently detailed in Ref. [2], significantly expands our theoretical understanding, particularly in devices incorporating topological effects.

[1] P. Zalom, M. Žonda and T. Novotný, arXiv:2310.02933 (2023).
[2] P. Zalom, Phys. Rev. B 108 (2023) 195123.

HL 15.5 Mon 17:45 H 3007

**Ground state topology of a four-terminal superconducting double quantum dot** — •Wolfgang Belzig[1], Lev Teshler[1], Hannes Weisbrich[1], Jonathan Sturm[2], Raffael Klees[3], and Gianluca Rastelli[4] — [1]Universität Konstanz — [2]Universität Würzburg — [3]Universität Augsburg — [4]CNR INO BEC Group Trento

In recent years, various classes of systems were proposed to realize topological states of matter. One of them are multiterminal Josephson junctions where topological Andreev bound states are constructed in the synthetic space of superconducting phases. Crucially, the topology in these systems results in a quantized transconductance between two of its terminals comparable to the quantum Hall effect. In this work, we study a double quantum dot with four superconducting terminals and show that it has an experimentally accessible topological regime in which the non-trivial topology can be measured. We also include Coulomb repulsion between electrons which is usually present in experiments and show how the topological region can be maximized in parameter space.
[1] L. Teshler, H. Weisbrich, J. Sturm, Raffael L. Klees, G. Rastelli, W. Belzig, SciPost Phys. 15 (2023) 214

HL 15.6 Mon 18:00 H 3007

**Nonmonotonic buildup of spin-singlet correlations in double quantum dot** — •Kacper Wrześniewski, Tomasz Ślusarski, and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Poland

Dynamical buildup of spin-singlet correlations between the two quantum dots is investigated by means of the time-dependent numerical renormalization group method. By calculating the time evolution of the spin-spin expectation value upon a quench in the hopping between the quantum dots, we predict a nonmonotonic buildup of spin-singlet state. In particular, we find that in short timescales the effective exchange interaction between the quantum dots is of ferromagnetic type, favoring spin-triplet correlations, as opposed to the long-time limit, when strong antiferromagnetic correlations develop and eventually an entangled spin-singlet state is formed between the dots. We also numerically determine the relevant timescales and show that the physics is generally governed by the interplay between the Kondo correlations on each dot and exchange interaction between the spins of both quantum dots.

This work was supported by the Polish National Science Centre from funds awarded through decisions No. 2017/27/B/ST3/00621 and No. 2022/45/B/ST3/02826. We also acknowledge the computing time at the Poznan Supercomputing and Networking Center.
[1] K. Wrześniewski, T. Ślusarski, I. Weymann, Rev. B 108 (2023) 144307.

## HL 16: Functional Semiconductors for Renewable Energy Solutions I

Time: Tuesday 9:30–11:45 Location: ER 325

HL 16.1 Tue 9:30 ER 325

**Metavalently bonded tellurides: the essence of improved thermoelectric performance in elemental Te** — •Yuan Yu[1], Decheng An[2], and Matthias Wuttig[1] — [1]Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany — [2]College of Chemistry, Taiyuan University of Technology, Taiyuan 030024, China

Doping is crucial to obtain high-efficiency elemental Te thermoelectrics. However, the remarkably low solubility of dopants such as As, Sb, and Bi in Te provides a major challenge. This also complicates the understanding of improved thermoelectric properties upon doping these elements. Here, we develop a correlative method to characterize the local microstructures and corresponding transport properties in doped Te crystals. We confirm that the conspicuous enhancement of bulk electrical conductivity and power factor stems from the dopant-induced formation of metavalently bonded precipitates, which form electrically beneficial interfaces with the Te matrix. A quantum-mechanical-derived chemical bonding map successfully uncovers efficient dopants for improving the thermoelectric performance of Te. Forming metavalently bonded tellurides, which facilitate charge transfer across the interface, becomes a key factor for property design. This nonclassical doping recipe is based on the newly developed understanding of the origins of thermoelectricity in this system and opens pathways for tailoring other complex semiconductors.

HL 16.2 Tue 9:45 ER 325

**Rational Design of the CoS Co9S8@NC Composite Enabling High-Rate Sodium-Ion Storage** — •Ying Qi — TU Ilmenau

Metal sulfides have been considered promising anode materials for sodium-ion batteries (SIBs) due to their high specific capacities. However, the poor electrical conductivity and sluggish electrochemical kinetics of metal sulfides are the critical factors that are limiting their applications. In this work, cobalt sulfides with heterostructures embedded in an N-doped carbon composite (CoS/Co9S8@NC) have been synthesized to further investigate Na+ diffusion in the SIBs. With contributions from the heterostructure, the N-doped carbon, and the unique morphology, the composite can deliver enhanced rate capability and cycling stability compared to Co9S8. This work depicts the change of Na+ diffusion under the influence of heterostructures, providing an effective strategy of material design for enhancing the electrochemical performance of sodium-ion storage.

HL 16.3 Tue 10:00 ER 325

**Constructing metal sulfide anodes with excellent K-ion storage properties via microstructure engineering** — •Kangzhe Cao[1,2], Huiqiao Liu[2], Jiahui Ma[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang 464000, China

K-ion batteries (KIBs) feathered by abundant resources and high energy densities are considered a kind of ideal candidates for the large-scale energy storage systems. Anode materials, such as metal sulfides, with high capacity always hold more than one K ions per molecule, companying large volume expansion during cycling. This character endangers the stability of the electrode structure and the solid-electrolyte-interphase (SEI) on the active materials, resulting in low coulombic efficiency and limited cycle life. Herein, we would like to introduce a strategy to construct a series of high-performance metal sulfide anodes for KIBs via structure engineering, including conversion reaction anodes and conversion-alloy reaction anodes. We will demonstrate how the confining layer improves the coulombic efficiency of CuS anode, why the electrochemical reversibility of Sb2S3 anode is triggered by the synergistic effect of confining and catalysis, and how to improve the cycling stability of SnS2 through heterostructure designing. Our work confirms that the K-ion storage properties of metal sulfide anodes can be largely improved by microstructure engineering, offering a reliable strategy for designing high-performance KIB anodes.

HL 16.4 Tue 10:15 ER 325

**Effects of Defects on the Optoelectronic Properties of $Ta_3N_5$ Thin Films** — •Lukas M. Wolz[1,2], Gabriel Grötzner[1,2], Laura I. Wagner[1,2], Tim Rieth[1,2], Matthias Kuhl[1,2], Guanda Zhou[1,2], Verena Streibel[1,2], Saswati Santra[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1,2] — [1]Walter Schottky Institute, Technische Universität München — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München

Photoelectrochemical (PEC) energy conversion is a promising approach for efficient solar-to-fuel conversion. In this context, transition metal nitride semiconductors have recently emerged as an interesting class of materials for overcoming the limitations associated with commonly studied metal oxides. While the impact of oxygen impurities ($O_N$) and nitrogen vacancies ($v_N$) on the PEC activity has already been explored, the understanding of how these defects impact stability is still lacking. Here, we utilize a controllable synthesis approach to independently tune $O_N$ and $v_N$ concentrations in $Ta_3N_5$ and systematically investigate structural, compositional, optoelectronic, and PEC properties to establish the relationship between atomic-scale defects and macroscale PEC stability. Low oxygen concentrations facilitate the formation of deep $v_N$ defects, leading to charge recombination and limiting the PEC stability. Increasing oxygen incorporation leads to the passivation of $v_N$ defects, resulting in reduced defect absorption, improved charge separation, and enhanced material stability. Overall, these results show the detrimental role of $v_N$ and the beneficial impact of $O_N$ on the stability of $Ta_3N_5$.

**15 min. break**

HL 16.5 Tue 10:45 ER 325

**Oxygen incorporation as a route to non-degenerate zinc ni-**

**tride** — •Elise Sirotti, Bianca Scaparra, Stefan Böhm, Felix Rauh, and Ian D. Sharp — Walter Schottky Institute and TUM School of Natural Sciences, Technical University of Munich

Zinc nitride ($Zn_3N_2$) comprises earth-abundant elements, possesses a small direct bandgap, and is characterized by high electron mobilities. These characteristics make it, in principle, a promising compound semiconductor for photovoltaic and thin-film transistor applications. However, in practice, the unintentional degenerate n-type doping that is commonly reported and often assigned to oxygen impurity doping significantly impedes its development for technological applications. To systematically investigate this doping effect, epitaxial $Zn_3N_2$ were grown by plasma-assisted molecular beam epitaxy with controlled oxygen content up to 20 at.% on a-plane sapphire, resulting in single phase (222)-oriented $Zn_3N_2$ with variable oxygen content. A combination of structural, electrical, and optical measurements reveals how, contrary to expectations, oxygen incorporation can lift the degenerate conductivity and achieve films with charge carrier concentrations in the $10^{17}\,cm^{-3}$ range. Indeed, both electrical and optical measurements confirm that the material changes from a degenerate metallic to semiconductor behavior as the oxygen content increases, suggesting the formation of charge-compensating defect complexes. The understanding of the beneficial role of oxygen thus provides a route to bring $Zn_3N_2$ into reach for technological applications.

HL 16.6 Tue 11:00 ER 325

**Cobalt nitride thin films for stabilizing nitride-based photoelectrodes** — •Matthias Kuhl[1,2], Lukas Kohlmaier[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

For artificial photosynthesis, metal nitride semiconductors evolved over recent years as a promising material class, offering narrow bandgaps that are ideal for visible light absorption and pronounced bond covalency that facilitates long range charge transport. However, these materials suffer from poor stability under realistic operation conditions. One strategy to improve stability is to interface the semiconductor light absorber with conformal and ultra-thin catalytic layers that still permit interfacial charge transport and minimize losses due to parasitic light absorption. In contrast to typically studied oxide protection layers, we use plasma-enhanced atomic layer deposition (PE-ALD) to deposit ultra-thin cobalt nitride films as conformal, stable, and catalytically active coatings. Different characterization techniques are combined to reveal the effect of varying synthesis parameters on the material properties. Explicitly, we demonstrate that the deposition temperature can be employed to tune the film composition and nitrogen content, thereby controlling the optoelectronic properties and catalytic activity. Overall, this work highlights the use of PE-ALD as a promising approach for engineering pure nitride catalyst/semiconductor interfaces to create efficient and stable photoelectrodes.

HL 16.7 Tue 11:15 ER 325

**Low temperature photoluminescence investigation of boron doped and quenched silicon** — •Kevin Lauer[1,2], Robin Müller[1], Zia Ul-Islam[1], Katharina Peh[1], Dirk Schulze[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

The linking of light-induced degradation (LID) with photoluminescence (PL) peaks has been shown to be very constructive in defect identification in case of indium doped silicon.[1] For boron doped silicon the search after PL peaks, which follow LID treatments, was not successful so far.[2] By applying quenching treatments[3] we were now able to discover a PL peak, which is impacted by LID treatments.[4] The relation of this discovered peak to closely neighbored known peaks is discussed.

[1] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, Phys. Status Solidi A, vol. 219, no. 19, p. 2200099, 2022 [2] K. Peh, K. Lauer, A. Flötotto, D. Schulze, and S. Krischok, Phys. Status Solidi A, vol. 219, no. 17, p. 2200180, 2022 [3] M. L. W. Thewalt, U. O. Ziemelis, and R. R. Parsons, Phys. Rev. B, vol. 24, no. 6, p. 3655, 1981. [4] K. Lauer et al., arXiv, Nov. 13, 2023. doi: 10.48550/arXiv.2311.07280.

HL 16.8 Tue 11:30 ER 325

**$CeTa(O,N)_3$ and $CeNb(O,N)_3$ perovskite oxynitrides for photoelectrochemical energy conversion** — •Gabriel Grötzner[1,2], Laura I. Wagner[1,2], Lukas Wolz[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

Photoelectrochemical (PEC) water splitting presents a promising avenue for the efficient storage of solar energy in chemical bonds. Perovskite oxynitrides, emerging as a new class of materials for PEC water splitting, hold potential to overcome certain limitations associated with more extensively studied metal oxides, particularly as many perovskite oxynitrides have a band gap of ∼2 eV. However, the optoelectronic properties of many perovskite oxynitrides are not well understood and investigated. This study introduces a novel method for synthesizing thin films of the perovskite oxynitrides $CeTa(O,N)_3$ and $CeNb(O,N)_3$ through a spin coating process followed by a two-step annealing procedure in ambient air and ammonia. The investigation explores the structural, compositional and optoelectronic properties of the thin films and furthermore compares the results between $CeTa(O,N)_3$ and $CeNb(O,N)_3$. Additionally, the influence of the annealing conditions in ammonia on the material properties is evaluated. The experimental findings unveil bandgaps in the visible range and n-type conductivity for both materials. As these results suggest use cases for both materials in PEC watersplitting, their viability as photoanodes is also evaluated.

## HL 17: Organic Semiconductors

Time: Tuesday 9:30–12:00 Location: EW 015

HL 17.1 Tue 9:30 EW 015

**Charge mobility in polar columnar phases of subphthalocyanine containing liquid crystals** — •Ahmad Murad[1], Elias Baron[1], Martin Feneberg[1], Maximilian Baumann[2], Matthias Lehmann[2], and Alexey Eremin[1] — [1]Otto-von-guericke-Universität — [2]Julius- Maximilians -Universität Würzburg

We report measurements of time-of-flight charge carrier mobility in star-shaped mesogens with subphthalocyanine core that forms self-assembled polar columnar phases. The study investigates the intricate interplay between temperature and electric field dependence on the high mobility of polar columnar phase liquid crystals (PCLCs). We demonstrate that the charge mobility exhibits an anomaleous field dependence decreasing with increasing electric field. PCLCs exhibit unique structural properties characterized by self-assembled columnar arrangements of mesogens with spontaneous polarisation, which make them promising candidates for various electronic and optoelectronic applications.

HL 17.2 Tue 9:45 EW 015

**Optical and electrically driven single-molecular Raman switch** — •Hai Bi — Jihua Laboratory, No.28 Huandao South road, Nanhai district, Foshan 528200, China

We have presented a single-molecular Raman switch, which is controlled not only by an applied voltage, but also by optical inputs with different directions. In this study, the combined effect of the near-field optical angular momentum and the bias voltage on the Raman response of a single molecular junction, creating a molecular switch, was investigated. It was demonstrated that the molecular switch can be manipulated using an optical input. The effects of both the polarisation of light and the subsequent symmetry properties of the electromagnetic near field were investigated and used to control the switching behaviour. This change in the Raman response of the junction is associated with a modification of the conformation of the molecule. By changing both the illumination side and the voltage applied to the junction, the Raman intensity can be turned ON and OFF with a difference of nearly five orders of magnitude between the two states.

HL 17.3 Tue 10:00 EW 015

**Isotope effects in Ga- and O-rich monoclinic $\beta$-$Ga_2O_3$** — •Daniel Cierpinsky[1], Benjamin M. Janzen[1], Andrea Ardenghi[2], Oliver Bierwagen[2], Piero Mazzolini[3], Roland Gillen[4], Janina Maultzsch[4], Andreas Falkenstein[5], Joe Kler[5], Roger Souza[5], Manfred Martin[5], and Markus R. Wagner[2,1] — [1]Technische Universität Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [3]University of Parma, Italy — [4]Chair of Experimental Physics, Erlangen, Germany — [5]RWTH Aachen University, Aachen, Germany

We employ polarization-dependent confocal micro-Raman spectroscopy to study the vibrational properties of isotopic $\beta$-$Ga_2O_3$. For this purpose samples were fabricated using molecular beam homoepitaxy to produce thin films of $^{18}O$ isotopic $Ga_2O_3$ on non isotopic $^{16}O$ $Ga_2O_3$ substrate, with growth conditions ranging from metal- to oxygen-rich regimes. We determine the spectral position of all Raman active phonon modes with high precision and observe that the substitution of $^{16}O$ with $^{18}O$ leads to shifts towards lower frequencies for all modes due to the higher isotopic mass. The isotopically induced shifts and their variations resulting from different growth regimes are discussed in conjunction with DFT calculations on the phonon energy contribution of lattice sites as well as SIMS measurements.

HL 17.4 Tue 10:15 EW 015

**Excitons in organic materials: Revisiting old concepts with new insights** — •S. Anhäuser[1], D. Bischof[1], A.M. Valencia[2], C. Cocchi[2], and G. Witte[1] — [1]Philipps-Universität Marburg, FB Physik — [2]Carl von Ossietzky Universität Oldenburg, FB Physik

The concept of excitons, originally developed for inorganic materials, is often directly transferred to organic materials, ignoring key differences in the properties of their optical excitations. Here we report a combined experiment/theory study carried out for acenes with focus on tetracene and perfluorotetracene, in order to critically examine these concepts. For this purpose we combine detailed optical spectroscopy of various states of matter ranging from solution, to poly- and single crystalline samples, and even melt, with state-of-the-art first-principles calculations, based on DFT and many-body methods on top. This integrated approach provides deep insights into the optical signatures of the organic systems and enables us to distinguish the single particle nature of excitations in isolated molecules from the collective nature of excitons in all aggregated phases. This shows that quantum mechanical interactions between similar molecules represent a critical link between these two scenarios [1]. Therefore, we propose to use the term 'exciton' only for optical excitations of aggregated molecular materials. The presented results not only provide a deeper understanding of the optical excitations in organic semiconductors, but also highlight roadmaps and potential pitfalls that need to be considered when studying these systems.

[1] A.M. Valencia et al., Electron. Struct. 2023, 5, 033003.

HL 17.5 Tue 10:30 EW 015

**Thermal Stability of Doped Organic Hole Transport Layers** — •Stephanie Buchholtz, Tobias Antrack, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden, Germany

The electrical conductivity of amorphous doped organic hole transport layers, as used in organic light-emitting diodes (OLEDs), solar cells or photodetectors, increases with temperature due to the dominant hopping-like transport mechanism. However, the conductivity breaks down irreversibly at a certain temperature. For example, OLEDs and organic photovoltaics have operating temperatures up to 80°C and 145°C, respectively. In addition, the active layer of an organic solar cell is deposited on the hole transport layer and has to be annealed at temperatures up to 140°C for a higher efficiency. The cause of the breakdown is unknown, which impedes the development of more stable devices. Here we show a relation between the breakdown of the conductivity and the glass transition of the small molecule host materials and find that the choice of the dopant and the doping concentration significantly affect the thermal stability of the layer. Based on our investigations, we develop different hypotheses about the cause of the breakdown. With our results, we devised strategies to improve the thermal stability of organic hole transport layers.

**15 min. break**

HL 17.6 Tue 11:00 EW 015

**Room-temperature polariton lasing and photonic confinement in an organic microcavity** — •Dominik Horneber[1], Johannes Düreth[1], Tim Schembri[2], Simon Betzold[1], Sven Höfling[1], Matthias Stolte[2], Frank Würthner[2], and Sebastian Klembt[1] — [1]Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg, Deutschland — [2]Center for Nanosystems Chemistry (CNC), Julius-Maximilians-Universität Würzburg, Theodor-Boveri-Weg, 97074, Würzburg, Deutschland

Perylene bisimides (PBIs) are organic dyes with quantum yields (PLQY) close to unity and excellent thermal and photo-chemical stability. These features as well as the tunability of their solid-state packing via chemical functionalization make this material class a promising candidate for lasing at room temperature. In this work, we show strong light-matter interaction and exciton-polariton lasing in optical microcavities with a neat layer of a PBI monomer that is shielded by voluminous bay-substituents to prevent aggregation-induced PLQY-quenching. Furthermore, photonic confinement in zero-dimensional resonators and chains of coupled resonators is demonstrated which shows the energetic discretization of the modes and the formation of a band-structure, respectively. This paves the way for the study of non-linear bosonic systems in artificial lattices hosting a highly stable PBI as solid-state emitter.

HL 17.7 Tue 11:15 EW 015

**Interplay of Electrical Conductivity and Seebeck Coefficient of n-doped NDI-based Polymer Thin Films for Thermoelectric Applications** — •Marie Siegert[1], Markus Hönig[2], Michael Sommer[2], and Jens Pflaum[1,3] — [1]University of Würzburg — [2]Chemnitz University of Technology — [3]CAE Bayern

Thermoelectric generators based on organic materials offer a sustainable, low-cost approach towards waste heat recovery and thus, efficient energy consumption. Disordered polymer thin films in particular exhibit aptly low thermal conductivties $\kappa$ for thermoelectric applications and their preparation via solution processing is easily scaled to meet industrial requirements. To improve their inherently low charge carrier concentration and therefore increase their electrical conductivity $\sigma$, suitable dopants can be employed. However, doping typically causes the Seebeck coefficent $S$ to decrease, and may even lead to a polarity change in $S$ at high doping concentrations, which is detrimental to thermoelectric efficiency. Here we conducted temperature dependent studies on thin films of the polymer PNDIT2 utilizing the n-type dopant TAM with regards to their thermoelectric properties. Systematically varying the molecular weight of the PNDIT2 host, the interplay of charge carrier density and mobility in this polymeric system and their effect on the Seebeck coefficient are revealed. The resulting power factors $PF = \sigma S^2$ suggest future strategies to further refine the doping protocol for polymer thin films and thus, to maximize their thermoelectric figure of merit. The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.

HL 17.8 Tue 11:30 EW 015

**Polymer-Metal-Composite Films with Structural Anisotropy for Thermoelectric Applications** — •Christian Gradl[1], Marie Siegert[1], and Jens Pflaum[1,2] — [1]Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]CAE Bayern, 97074 Würzburg

To address the intrinsic limitations of neat organic semiconductors in thermoelectric (TE) applications, the fabrication of composites offers a promising approach by synergizing the best properties of the individual components. Inducing spatial order within such composite films can further enhance their TE performance. We applied this concept to the crystalline 1D molecular p-type metal $TTT_2I_3$ which has intriguing potential for TE applications due to its high electrical and low thermal conductivity. Our research focuses on exploiting these TE properties in conjunction with the anisotropic spatial orientation of the microcrystals within PEDOT:PSS polymer films. The $TTT_2I_3$ crystals are grown by microspacing in-air sublimation on single crystal RbCl substrates under ambient conditions. The self-alignment of the microcrystals originates from the growth on the respective RbCl surface facet and, hence, can be modified by the specific choice of a certain surface orientation. Subsequently, the aligned $TTT_2I_3$ microcrystals were enclosed by a solution processed p-type conducting PEDOT:PSS layer to finalize the composite thin film preparation. By the analysis of the thermoelectric properties, we are able to highlight the role of the 1D organic metal additives and their anisotropic spatial alignment on the TE characteristics of the polymer-metal composite films.

HL 17.9 Tue 11:45 EW 015

**Direct observation of the energy band structure of the super atom molecular orbital in solid phase C60** — •Daichi Homma[1], Susumu Yanagisawa[2], and Hiroyuki Yoshida[1,3] — [1]Graduate School of Engineering, Chiba University, Chiba, Japan — [2]Faculty of Science, University of the Ryukyus, Okinawa, Japan — [3]Chiba University MCRC, Chiba, Japan

The Super Atom Molcular Orbital (SAMO) is a hydrogen-like unoccupied orbital in which an electron is loosely bound around a central Coulomb potential of a molecule. Because of this nature, SAMO is predicted to form nearly free electron (NFE) bands in solids, which should exhibit high electron mobility. SAMO was first observed in C60 [1] and has so far only been observed in the monolayer and in the gas phase. To discuss the electron mobility in the solid phase, it is essential to detect the SAMO and measure the band structure in the solid state.

Recently, we have developed angle-resolved low-energy inverse photoelectron spectroscopy [2]. Using this technique, we observed the s-SAMO of C60 in bulk for the first time and further revealed the band structure. We prepared a 10 nm thick epitaxially grown C60 film on the Cu(111). From the comparison with the previous studies, we assigned a peak 2.97eV above the LUMO band as the SAMO-derived band. The observed band structure is NFE-like with an effective mass of 1.35 me. [1] M. Feng, et al., Science 320, 359 (2008). [2] Y. Kashimoto, et al., Rev. Sci. Instrum. 94, 063903 (2023).

## HL 18: 2D Materials and Heterostructures: Emerging Materials and Phenomena

Time: Tuesday 9:30–13:00 Location: EW 201

HL 18.1 Tue 9:30 EW 201

**Quantum transport in monolayer and multilayer Black Phosphorene** — Jouda J. Khabthani[1], Khouloud Chika[1], Ghassen Jemaï[1], Didier Mayou[2], and •Guy Trambly de Laissardière[3] — [1]Lab. de Physique de la Matière Condensée, Faculté des Sciences de Tunis, University El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS / Univ. Grenoble Alpes, Grenoble, France — [3]Lab. de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, Cergy-Pontoise, France

The electronic properties of Phosphorene are very sensitive to local defects such as fonctionalization which may be covalent (resonant) or non-covalent (non-resonant). Here, we present numerical studies on the electronic structure and quantum transport in monolayer Black Phosphorus (BP), few-layer BP, and bulk BP, with a relatively high concentration of defects (a few %). In contrast to the usual Boltzmann approach for electronic transport calculations, our real space method [1,2] takes into account all the effects of defects on the electronic structure itself and the impacts of multiple scattering on conductivity. Our study shows that resonant and non-resonant scatterers have different consequences on the gap and conductivity, sometimes leading to metal-insulator transitions by varying the defect concentration.

[1] F. Triozon *et al.*, Phys. Rev. B **65**, 220202, (2002).

[2] G. Trambly de Laissardière, D. Mayou, Phys. Rev. Lett. **111**, 146601 (2013).

HL 18.2 Tue 9:45 EW 201

**Influence of highly charged ion irradiation on the electrical and memory properties of black phosphorus field-effect transistors** — •Stephan Sleziona, Osamah Kharsah, Lucia Skopinski, Leon Daniel, Jennifer Schmeink, and Marika Schleberger — Fakultät für Physik und CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47057 Duisburg, Germany

Black phosphorus (bP) is one of the more recently discovered layered materials. In particular its high hole mobility and finite, thickness dependent, direct bandgap may pave its way to new applications as optoelectronic devices. Utilizing the hysteresis in the transfer characteristics of bP field-effect transistors (FETs), several approaches to realize non-volatile memory devices have been successfully put forward. This hysteresis is commonly attributed to charge trapping and detrapping in defects and impurities either in the underlying substrate, or in the bP itself. In this work we deliberately introduce additional defects into bP FETs by irradiating the devices with highly charged $Xe^{30+}$ at a kinetic energy of 180 keV to manipulate the electrical and memory properties of the devices. We find an increase of conductivity and p-doping with increasing ion fluence, while other device parameters, like i.e. charge carrier mobility, degrade for the higher irradiation fluences. Most importantly, we find an increase in the width of the hysteresis and the memory window due to the irradiation. By controlling the kinetic energy of the ions, we can demonstrate, that this increase is caused by additional defects in the underlying $SiO_2$ substrate and not in the bP itself.

HL 18.3 Tue 10:00 EW 201

**On-site Coulomb energy in TMDC compounds** — •Yashasvi Mehra[1,2,3], Samuel Bealieu[4], Mauro Fanciulli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Marcin Rosmos[5], Natalia Olszowska[5], Aki Ismo Olavi 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]Université de Bordeaux, CNRS, CEA, CELIA, UMR5107, Talence, France — [5]SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland

The Coulomb interaction U, serves as a pivotal parameter influencing electron behavior, particularly accentuated within low-dimensional materials. Transition Metal Dichalcogenides, quasi-2-D systems, exhibit diverse electronic traits like CDW order, co-existing CDW with superconductivity, and topologically non-trivial phases. Their 2D nature intensifies electron-coulomb interaction, leading to phenomena like Mott-Hubbard transitions. We aim to determine the on-site Coulomb interaction for each element within two series of TMDC materials (MX2, where X = S, Se, Te, M = Nb, Ta) by resonant ARPES.

HL 18.4 Tue 10:15 EW 201

**Tuning properties of 2D Janus MoSSe** — •Jennifer Schmeink, Jens Osterfeld, Osamah Kharsah, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Two-dimensional (2D) Janus materials such as MoSSe are defined by their asymmetrical structure, where the transition metal atoms, specifically molybdenum (Mo), are sandwiched between opposing sites of different species of chalcogen atoms, notably selenium (Se) and sulfur (S). This uniquely structured material allows a new way for tuning existing properties of 2D transition metal dichalcogenide (TMDC) materials and new characteristics emerge from the loss of inversion symmetry in the structure.

The method for synthesizing such Janus materials involves utilizing a base TMDC, e.g. molybdenum diselenide ($MoSe_2$). The process involves the creation of vacancies in the top layer of chalcogen atoms, subsequently filling these vacancies with an additional species [1]. Depending on the process details, this results in Janus MoSSe or in Janus-like $MoS_{2(1-x)}Se_{2x}$ alloys, where $0 > x > 1$ and $x \neq 0.5$. The latter is characterized by the coexistence of Janus MoSSe and $MoSe_2$ or $MoS_2$ phases. This constitutes yet another tunable platform for tailoring material properties.

This talk will present studies of the (opto-)electronic properties of Janus MoSSe and its Janus-like alloys. Furthermore, the influence of Se-vacancies in $MoSe_2$ and the Janus-like alloys will be highlighted and defect related findings discussed.

[1] J. Schmeink *et al.*, Nanoscale (2023), **15**, 10834-10841

HL 18.5 Tue 10:30 EW 201

**$PtSe_2$ vdW single-crystal surfaces studied at the atomic scale with ncAFM** — •Igor Sokolović[1,2], Saeed Rasouli[2], Bing Wu[3], Zdeněk Sofer[3], Aleksandar Matković[4], Michael Schmid[2], Ulrike Diebold[2], and Tibor Grasser[1] — [1]Institute of Microelectronics, TU Wien, Vienna, Austria — [2]Institute of Applied Physics, TU Wien, Vienna, Austria — [3]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague, Czech Republic — [4]Chair of Physics, Montanuniversität Leoben, Leoben, Austria

Surfaces of van-der-Waals-bonded (vdW) single-crystal $PtSe_2$ cleaved in ultrahigh vacuum (UHV) were studied with noncontact atomic force

microscopy (ncAFM) at the atomic level. Typical ionic and electronic defects were characterized with single-atom precision: the identification of surface and subsurface defects was achieved by observing the atomic and electronic structure in parallel. The metallic single crystals exhibit a proclivity of the PtSe2 toward different defect types compared to the synthesized trilayer thin films of semiconducting $PtSe_2$ and other Pt-based TMDs. Cleaved surfaces are representative of the commonly exfoliated flakes so further experiments with *in situ* deliberate stoichiometry adjustments and the adsorption of gasses will be presented. Additionally, the growth of a $CaF_2$ dielectric on these surfaces will be demonstrated.

HL 18.6 Tue 10:45 EW 201

**Nanoscale Charge Transport Characterization of Novel Type 2D MOFs and COFs** — •Jonas Pöhls[1], Zhiyong Wang[2,3], Laura Frey[4], Renhao Dong[2], Dana Medina[4], Xinliang Feng[2,3], and Thomas Weitz[1] — [1]1st Institute of Physics, University of Goettingen, Goettingen, Germany — [2]Chair of Molecular Functional Materials, TU Dresden, Germany — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Chemistry Department, LMU Munich, Germany

In recent years, Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have emerged as fascinating and promising materials classes, owing to their exceptional structural versatility and tunable properties, which make them interesting for a wide range of technological applications. At the same time, the study of 2D van der Waals materials has become the probably most relevant and dynamic area in solid state research at present, offering numerous opportunities to uncover novel physical phenomena and engineer advanced nanoscale devices. With recent advances in the synthesis of two-dimensional MOFs and COFs, these material classes have also entered the field of van der Waals materials [1]. We will characterize the charge transport in novel type 2D coordination network materials like Cu-BHT, considering also the influence of properties like structure or defects. By that, we will demonstrate why they are promising candidates for implementation into van der Waals heterostructures.

**15 min. break**

HL 18.7 Tue 11:15 EW 201

**Srain control of exciton and trion spin-valley dynamics in monolayer transition metal dichalcogenides** — Zhao An[1], Pedro Soubelet[2], Yaroslav Zhumagulov[3], Michael Zopf[1], •Alex Delhomme[2], Chenjiang Qian[2], Paulo Faria Junior[3], Jaroslav Fabian[3], Xin Cao[1], Jingzhong Yang[1], Andreas Stier[2], Fei Ding[1], and Jonathan Finley[2] — [1]Institute of Solid State Physics, Leibniz Universitat Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Walter Schottky Institut and TUM School of Natural Sciences, Technische Universitat Munchen, Am Coulombwall 4, 85748 Garching, Germany — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany.

The electron-hole exchange interaction is a fundamental mechanism that drives valley depolarization via intervalley exciton hopping in semiconductor multivalley systems. Here, we report polarization-resolved photoluminescence spectroscopy of neutral excitons and negatively charged trions in monolayer MoSe2 and WSe2 under biaxial strain. We observe a marked enhancement (reduction) on the WSe2 triplet trion valley polarization with compressive (tensile) strain while the trion in MoSe2 is unaffected. The origin of this effect is shown to be a strain-dependent tuning of the electron-hole exchange interaction. A combined analysis of the strain-dependent polarization degree using ab initio calculations and rate equations shows that strain affects intervalley scattering beyond what is expected from strain-dependent band-gap modulations. The results evidence how strain can be used to tune valley physics in energetically degenerate multivalley systems.

HL 18.8 Tue 11:30 EW 201

**Strain fingerprinting of exciton valley character in 2D semiconductors** — •Abhijeet Kumar[1], Denis Yagodkin[1], Roberto Rosati[2], Douglas J. Bock[1], Christoph Schattauer[3], Sarah Tobisch[3], Joakim Hagel[4], Bianca Höfer[1], Jan N. Kirchhof[1], Pablo H. López[5], Kenneth Burfeindt[1], Sebastian Heeg[5], Cornelius Gahl[1], Florian Libisch[3], Ermin Malic[2], and Kirill I. Bolotin[1] — [1]Free Universität Berlin, Germany — [2]Philipps-Universität Marburg, Germany — [3]TU Wien, Austria — [4]Chalmers University of Technology, Sweden — [5]Humboldt-Universität Berlin, Germany

Momentum-indirect excitons define optoelectronic properties of many 2D semiconductors, but are challenging to detect due to their weak coupling to light. The identification of the excitons' valley character is further limited by complexities associated with momentum-selective probes. Here, we study the photoluminescence of controllably strained 2D materials at cryogenic temperatures and find that indirect excitons i) exhibit valley-specific energy shifts, enabling their valley fingerprinting, and ii) hybridize with bright excitons, becoming directly accessible to optical spectroscopy methods. This approach allows us to identify multiple previously inaccessible excitons with wavefunctions residing in K, Γ, or Q valleys in the momentum space, as well as various types of defect-related excitons. Overall, our approach is well-suited to unravel and tune intervalley excitons in various 2D systems.

HL 18.9 Tue 11:45 EW 201

**Strain control of hybridization between dark and localized excitons in a 2D semiconductor** — •Pablo Hernández López[1], Sebastian Heeg[1], Christoph Schattauer[2], Sviatoslav Kovalchuk[3], Abhijeet Kumar[3], Douglas J. Bock[3], Jan N. Kirchhof[3], Bianca Höfer[3], Kyrylo Greben[3], Denis Yagodkin[3], Lukas Linhart[2], and Florian Libisch[2] — [1]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Vienna University of Technology, Vienna, Austria — [3]Physics Department, Freie Universität Berlin, Berlin

Mechanical strain is a powerful tuning knob for excitons, Coulomb-bound electron-hole complexes dominating optical properties of two-dimensional semiconductors. While the strain response of bright free excitons is broadly understood, the behaviour of dark free excitons (long-lived excitations that couple weakly with light due to conservation laws) or localized excitons related to defects remains mostly unexplored. Here, we study the strain behaviour of these fragile many-body states on pristine suspended WSe2 kept at cryogenic temperatures. We find that upon straining, dark and localized excitons in monolayer WSe2 are brought into energetic resonance, forming a new hybrid state that inherits the properties of the constituent species. The characteristics of the hybridized state, including an order-of-magnitude enhanced light/matter coupling, avoided-crossing energy shifts, and strain tunability of many body interactions, are all supported by first-principles calculations. The hybridized exciton reported here may play a critical role in the operation of single quantum emitters based on WSe2.

HL 18.10 Tue 12:00 EW 201

**Electronic effects on wrinkled 2D TMDCs** — •Mohammadreza Daqiqshirazi and Thomas Brumme — Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstraße 66c, 01069 Dresden, Germany

Strain can be used to change the electronic properties of 2D materials considerably especially since they can undergo strong deformations before breaking. It has been shown that there are various techniques to create wrinkles or folds in 2D materials. The wrinkles exert an inhomogeneous strain field on the 2D material that goes beyond the conventional uniaxial and biaxial strain effects. It is very important to understand these effects as wrinkles and bubbles can also occur during the synthesis or due to the transfer process. Unfortunately, these inhomogeneous strains are rarely studied using fundamental methods because the size of the systems is enormous. Here we investigate the effect of an inhomogeneous strain field in the form of wrinkles in 2D WSe2 monolayers, bilayers and heterostructures of WSe2-MoSe2. We use density functional theory and include spin-orbit coupling in our calculations. We find that spin-orbit coupling and symmetry breaking in monolayers lead to a strong Rashba-like splitting. Furthermore, from the band structures, we can explain the localization of the excitons in certain regions of the systems due to strain fields.

HL 18.11 Tue 12:15 EW 201

**Extended suspension of transition metal dichalcogenide monolayers** — •Leonard Geilen[1,3], Lukas Schleicher[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

Suspended 2D materials offer great possibilities in the realm of investigating the fundamentals of nano- and micromechanical systems as well as chip-based sensors. So far, 2D materials have been suspended on the order of tens of micrometers in the case of few-layer materials and up to ten for monolayers. We demonstrate how a dry-transfer allows fabricating suspended monolayers of transition metal dichalcogenides

with diameters larger than ten micrometers and a reduced impact of fabrication residues.

HL 18.12 Tue 12:30 EW 201

**Impact of atomic layer deposition growth rate on the properties of $MoS_2$ and $WS_2$** — •Christian Tessarek, Tim Grieb, Florian F. Krause, Christian Petersen, Alexander Karg, Alexander Hinz, Niels Osterloh, Christian Habben, Stephan Figge, Andreas Rosenauer, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

The direct band gap of monolayer $MoS_2$ and $WS_2$ enables the use of these layers in optoelectronic applications. To overcome the limited and random size of exfoliated flakes from bulk material, chemical vapor deposition (CVD) techniques are necessary to grow homogeneous layers on large substrates.

Atomic layer deposition, a modified CVD method using an alternating precursor supply at lower process temperature, was used to grow $MoS_2$ and $WS_2$ on $SiO_2$/Si substrates. The growth rate is identified as a major parameter that influences the optical and structural properties. Raman spectroscopy investigations were carried out to characterize the 2D layers. Monolayers only form applying a slow growth rate. For a fast growth rate multilayers with minor structural properties directly develop in the initial phase. The optical activity was demonstrated by photoluminescence measurements which show typical A and B excitonic emission for $MoS_2$ and $WS_2$ monolayers. Further studies by X-ray photoelectron spectroscopy and transmission electron microscopy were carried out to reveal the stoichiometry and crystalline quality of the layers.

HL 18.13 Tue 12:45 EW 201

**Oxidative chemical vapor deposition of highly conductive and transparent polymer layers for contact fabrication in 2D-$MoS_2$-based FET structures** — •Jinmei Zhu[1,3], Florian Meierhofer[1], Marius Eckert[1,2], Stefan Wundrack[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology (IHT), TU Braunschweig, Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [3]Shijiazhuang College of Applied Technology, Shijiazhuang, China

For 2D $MoS_2$ field-effect transistors (FETs), contact fabrication easily results in damaging the $MoS_2$ channel due to the fragility of the atomically thin structure, making it difficult to reliably achieve high-performance devices. To overcome this challenge, the deposition of highly conductive and transparent polymer layers from the gas phase (oxidative chemical vapor deposition (oCVD)), is a promising approach that can lead to low-defect Ohmic contacts. In this work, we fabricated 2D $MoS_2$ bottom-gated FETs with poly (3, 4- ethylenedioxythiophene) (PEDOT) electrodes. PEDOT is a conductive polymer widely used as a transparent electrode material. We developed two contacting strategies to achieve a low-defect interface: in-situ oCVD electrode growth and electrode transfer method. By these means, we could pattern PEDOT layers and contact them onto $MoS_2$ channels without aggressive chemical and physical treatments. This allowed us to achieve low-defect $MoS_2$ channels with a clean and smooth interface of the PEDOT electrodes, significantly decreasing the charged impurity and interface-roughness scattering processes.

## HL 19: Quantum Dots and Wires: Optics I

Time: Tuesday 9:30–13:00 Location: EW 202

HL 19.1 Tue 9:30 EW 202

**Dynamics of Robust Photonic Cluster-State Generation from Quantum-Dot Molecules** — •David Bauch, Nikolas Köcher, Nils Heinisch, and Stefan Schumacher — Physics Department, CeOPP, and PhoQS, Paderborn University, Germany

Quantum Dot Molecules (QDMs) have garnered significant attention for their role in measurement-based quantum computation and communication, specifically due to their ability to generate indistinguishable and temporally strongly entangled photon states [1]. Recent theoretical strides have advanced methods for generating these states across various physical systems. Within the intrinsically emerging lambda systems in QDMs, rotations and excitations between the ground states facilitate photon generation, contributing to the formation of cluster states, photonic graph states, and beyond [1,2]. Our research focusses on the generation of simple linear cluster states from QDMs. We demonstrate temporal dynamics, strong correlations, time-bin entanglement through stabilizer generator expectation values and indistinguishability among emitted photons. Our numerical exploration provides detailed insights into the efficiency and viability of the emission protocol for the deterministic generation of highly entangled photonic cluster states. This serves as a crucial steppingstone for advancing the generation of more intricate states such as higher dimensional photonic cluster and graph states, marking a noteworthy step towards the utilization of photonic quantum states in practical applications.

[1] Vezvaee et al., Phys. Rev. Appl. 18.L061003 (2022). [2] Raissi et al., arXiv preprint 2211.13242 (2022)

HL 19.2 Tue 9:45 EW 202

**Magneto-optical generation and characterization of dark exciton state in a quantum dot** — •René Schwarz[1], Florian Kappe[1], Yusuf Karli[1], Thomas Bracht[2], Saimon Covre da Silva[3], Armando Rastelli[3], Vikas Remesh[1], Doris Reiter[2], and Gregor Weihs[1] — [1]Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria — [2]Condensed Matter Theory, Department of Physics, TU Dortmund, Dortmund, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria

Semiconductor quantum dots are arguably the most promising platform for future quantum technologies. Due to the confinement of charge carriers, a variety of photon states can be generated, making them a highly adaptable quantum platform. While the most common optical excitation methods target the so-called bright excitons or biexcitons for the generation of single or entangled photon states, quantum dots also accommodate optically dark excitons, which are not directly accessible via optical excitation methods. The dark exciton states exhibit significantly slower decay rates compared to their bright counterparts, making them potential candidates for application in quantum information protocols that demand the control of quantum coherence over long time scales [1]. In this work, we generate the dark exciton states in a single GaAs/AlGaAs quantum dot emitting ~ 800 nm under a magneto-optical excitation (in-plane magnetic field ~ 3.2 T), and characterize the emission energy splitting, lifetime variation and polarization response. [1] Phys. Rev. Lett. 94, 030502 (2005)

HL 19.3 Tue 10:00 EW 202

**Stimulated excitation and coherent control of dark exciton state population in a quantum dot** — •Florian Kappe[1], René Schwarz[1], Yusuf Karli[1], Thomas Bracht[2], Saimon Covre da Silva[3], Armando Rastelli[3], Vikas Remesh[1], Doris Reiter[2], and Gregor Weihs[1] — [1]Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria — [2]Condensed Matter Theory, Department of Physics, TU Dortmund, Dortmund, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria

Semiconductor quantum dots, with their capability of confining charge carriers and various spin configurations resulting from it, can be regarded as a highly versatile platform for generating non-classical light. While the generation of single photons or entangled photon pairs from quantum dots utilizes the so-called bright excitons and biexcitons respectively, quantum dots can also host optically dark excitons. Such states are optically inactive due to the spin-selection rules. Due to their longer coherence times, a direct and coherent optical excitation and control of dark states are of great interest in modern quantum information protocols [1]. In this work we demonstrate a stimulated excitation and coherent control of the dark exciton population via the biexciton state in a GaAs/AlGaAs quantum dot in presence of an in-plane magnetic field. The versatility of our scheme allows not only a deterministic preparation, but storage and a temporal retrieval of the dark state population, giving rise to a programmed single photon/photon pair emission.

HL 19.4 Tue 10:15 EW 202

**Coherent Preparation of High Quality Single Photon States**

— •Yusuf Karli[1], Florian Kappe[1], Ria G. Krämer[2], René Schwarz[1], Thomas K. Bracht[3], Daniel Richter[2], Doris E. Reiter[3], Stefan Nolte[2], Gregor Weihs[1], and Vikas Remesh[1] — [1]Institut für Experimentalphysik, Universität Innsbruck, 6020, Innsbruck, Austria — [2]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Center of Excellence in Photonics, 07745 Jena, Germany — [3]Condensed Matter Theory, Department of Physics, TU Dortmund, 44221 Dortmund, Germany

Traditional Two-Photon Excitation (TPE) methods not only face challenges related to indistinguishability and photon number coherence but also exhibit sensitivities to the excitation laser pulse parameters. In response, we introduce a Stimulated Two-Photon Excitation (sTPE) within Adiabatic Rapid Passage(ARP) process , where a second laser pulse resonant with the biexciton-to-exciton transition significantly reduces time jitter, enhancing both indistinguishability and photon number coherence. Experimental results demonstrate the effectiveness of sTPE within Adiabatic Rapid Passage (ARP) schemes, offering a promising avenue for robust single-photon generation to advance quantum communication technologies.

HL 19.5 Tue 10:30 EW 202

**Electron capture dynamics into self-assembled quantum dots far from equilibrium with their environment** — •Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Arne Ludwig[2], and Andreas Dirk Wieck[2] — [1]Heinrich-Heine Universität, Düsseldorf, Germany — [2]Ruhr-Universität, Bochum, Germany

The electron capture process in self-assembled quantum dots at large distance from the reservoirs is studied by deep level transient spectroscopy. Capture rates are obtained as a function of temperature, applied bias voltage and quantum dot occupancy. The observed activated character of the capture suggests that the back contact is the dominant electron source. A model is developed where electrons diffuse from the reservoir across the barrier onset from the space charge region to be captured by the self-assembled quantum dots.

HL 19.6 Tue 10:45 EW 202

**Entanglement in Resonance Fluorescence** — •Santiago Bermúdez Feijóo[1], Juan Camilo Lopez Carreño[2], and Magdalena Stobinska[3] — [1]Departamento de Fisica, Universidad Nacional de Colombia, Ciudad Universitaria, K. 45 No. 26 85, Bogota D.C., Colombia — [2]Institute of Theoretical Physics, University of Warsaw, ul. Pasteura 5, 02-093, Warsaw, Poland — [3]Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, ul. Banacha 2, 02-097 Warsaw, Poland

Particle entanglement is a fundamental resource upon which are based many quantum technologies. In this Article, we introduce a new source of entangled photons based on resonance fluorescence delivering photon pairs as a superposition of vacuum and the Bell state $|\Phi-\rangle$. Our proposal relies on the emission from the satellite peaks of a two-level system driven by a strong off-resonant laser, whose intensity controls the frequencies of the entangled photons. Notably, the frequency of the entangled photons can be tuned without decreasing their degree of entanglement and, unlike current technologies, the intensity of our source can be increased without the risk of spoiling the signal by involving high-order processes into the emission. Finally, we illustrate the power of our novel source by exciting an ubiquitous condensed-matter system, namely polaritons, and showing that they are left in a maximally entangled steady state.

**30 min. break**

HL 19.7 Tue 11:30 EW 202

**Temperature-independent photon entanglement from quantum dots** — •Thomas Bracht[1,2], Moritz Cygorek[3], Tim Seidelmann[4], Vollrath Martin Axt[4], and Doris E. Reiter[2] — [1]Institut für Festkörpertheorie, Uni Münster, DE — [2]Condensed Matter Theory, TU Dortmund, DE — [3]Heriot-Watt University, Edinburgh, UK — [4]Theoretische Physik III, Universität Bayreuth, DE

High levels of entanglement are essential for reliable quantum communication. In this context, quantum dots have emerged as a promising platform, offering excellent photon properties and controllability.

Here, I propose a novel approach to achieve maximal entanglement, overcoming previous shortcoming for example in two-photon excitation. Building upon the Swing-Up of Quantum Emitter (SUPER) scheme, I demonstrate its efficiency in generating entangled photon pairs from quantum dot systems in optical cavities [1]. An important aspect of this approach is the decoupling of the preparation process from the subsequent photon emission, enabling an effective initial-value problem, previously inaccessible in two-photon absorption settings. By leveraging this decoupling, an entanglement with unprecedentedly high fidelity is achieved, even when accounting for phonon interaction at elevated temperatures up to 80K. This makes the approach interesting for the use in real-world quantum communication scenarios.

[1] T. K. Bracht et al., Optica Quantum (accepted, 2024)

HL 19.8 Tue 11:45 EW 202

**Development and deterministic fabrication of electrically controlled quantum dot bullseye resonators** — •Setthanat Wijitpatima[1], Priyabrata Mudi[1], Avijit Barua[1], Normen Auler[2], Binamra Shrestha[2], Sven Rodt[1], Dirk Reuter[2], and Stephan Reitzenstein[1] — [1]Institute of Solid-State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Center of Optoelectronics and Photonics, Paderborn University, Warburger Str. 100, 33098 Paderborn, Germany

Quantum repeaters hold the potential to contribute to long-distance quantum communication significantly. They can be made of such quantum light sources with high photon extraction efficiency (PEE), high single-photon purity, high indistinguishability, and precise control over spectral features. We present a new device design enabling the electrical control of quantum dots (QDs) by deterministically integrating them into electrically connected bullseye resonators. Numerical simulations are conducted to optimize both the epitaxial layer structure and the nanophotonic device design achieving a high PEE of 74% at a numerical aperture of 0.8. Marker-based cathodoluminescence scans are performed to pre-select suitable QDs, which are then pre-characterized via electric-field-dependent microphotoluminescence measurements before electron beam lithography is performed to fabricate QD-bullseye resonators. After the integration, the post-characterizations are carried out on the same QDs to study the effect of device fabrication on their electro-optical properties.

HL 19.9 Tue 12:00 EW 202

**Swing-Up Dynamics in Quantum Emitter Cavity Systems: Near Ideal Single Photons and Entangled Photon Pairs** — •Nils Heinisch, Nikolas Köcher, David Bauch, and Stefan Schumacher — Physics Department, CeOPP, and PhoQS, Paderborn University, Germany

In the SUPER scheme (Swing-UP of the quantum EmitteR population) excitation of a quantum emitter is achieved with two off-resonant, red-detuned laser pulses, as theoretically [1] and experimentally demonstrated [2,3]. In particular, this approach promises generation of high-quality single photons without the need of complex laser stray light suppression or careful spectral filtering. In the present work we extend this method to quantum emitters, specifically semiconductor quantum dots (QDs), inside a resonant optical cavity [4-6]. A significant advantage of the SUPER scheme is identified in that it eliminates re-excitation of the quantum emitter by suppressing photon emission during the excitation cycle via the AC-Stark effect. This, in turn, leads to almost ideal single photon purity, overcoming a major factor typically limiting the quality of photons generated with quantum emitters in high quality cavities. We further find that for cavity-mediated degenerate photon-pair generation from the QD biexciton the SUPER excitation does not spoil the polarization entanglement. [1] T. K. Bracht et al., PRX Quantum 2, 040354 (2021). [2] Y. Karli et al., Nano Letters 22, 6567 (2022). [3] K. Boos et al., arXiv:2211.14289 (2022). [4] N. Heinisch et al., arXiv:2303.12604 (2023). [5] L. Vannucci et al., PRB 107, 195306 (2023). [6] T. K. Bracht et al., arXiv:2307.00304 (2023).

HL 19.10 Tue 12:15 EW 202

**Deterministic nanofabrication of Purcell-enhanced single-photon sources based GaAs quantum dots** — •Dinara Basharova[1], Nand Lal Sharma[2], Ching-Wen Shih[1], Chirag Palekar[1], Alexander Kosarev[1], Sven Rodt[1], Sai Abhishikth Dhurjati[2], Caspar Hopfmann[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, 01069 Dresden, Germany

On-demand single-photon and entangled photon pair sources based on semiconductor quantum dots (QDs) have drawn a great attention in the applications of quantum technologies, including quantum networks and computation. In quantum communication networks, quantum re-

peaters with QDs are necessary to extend the range of communication distance. In our work, we deterministically integrate semiconductor heterostructures with high-quality GaAs quantum dots emitting at 780 nm into circular Bragg grating (CBG) resonators with a gold mirror. Our design exhibits a theoretical photon extraction efficiency above 70% and a Purcell factor exceeding 14. In addition, in combination with reflectance measurement, we optimize the fabrication process to achieve excellent cavity performance. We use marker based electron beam lithography (EBL) as precise deterministic nanofabrication technique. The fabricated quantum light sources are characterized by high-resolution cathodoluminescence, micro-photoluminescence, and quantum optical spectroscopy, showing multi-photon emission suppression with g(2)(0) = 93%.

HL 19.11 Tue 12:30 EW 202

**Quantum optical properties of resonantly excited semiconductor quantum dots embedded in hybrid circular Bragg Gratings** — •Martin von Helversen[1], Lucas Rickert[1], Daniel Vajner[1], Johannes Schall[1], Shulun Li[1,2], Sven Rodt[1], Zhichuan Niu[2], Stephan Reitzenstein[1], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technical University Berlin, Berlin, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China

Aiming at the efficient on-demand generation of indistinguishable and highly pure single-photons, semiconductor quantum dots have proven excellent candidates - to large extend also due to the vast progress in their integration into photonic cavities. Amongst these, hybrid circular Bragg Gratings (hCBGs) have quickly become a well established choice, due to their broad outcoupling enhancement combined with high Purcell factors. Owed to the possible generation of polarization entangled photons, much research focuses on two-photon-resonant excitation.
In this work, we take advantage of a deterministically integrated QD in a hybrid CBG with a $T_1$-time below 50 ps to study its quantum optical properties under quasi-resonant p-shell as well as resonant s-shell excitation, the latter in continuous wave as well as in the pulsed regime under varying optical pulse-lengths. While purities exceeding 98% are achieved even under p-shell, we observe indistinguishable photons with a non-postselected visibility of over 88% under resonant excitation.

HL 19.12 Tue 12:45 EW 202

**Highly coherent GaAs-based microcavity polaritons dots at 200 K** — •Ismael dePedro-Embid, Alexander Kuznetsov, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

Microcavity (MC) polaritons, serve as an exceptional bridge between condensed matter and photonic systems. Achieving precise control over their spatial distribution, stability, and coherence is crucial for unlocking their full potential in practical applications. This can be achieved by creating zero-dimensional polariton dots by lateral confinement within the MC spacer. In this study, we investigate the effects of lateral confinement on the energy and temporal coherence of MC polaritons in (Al, Ga) As intracavity dots at temperatures up to 200 K, which are much higher than the usually studied temperatures of around 10 K for this material system. Our experimental results show that the spectral linewidths of the confined polariton states are substantially narrower than their unconfined counterparts, demonstrating that confinement significantly enhances the temporal coherence across a broad range of dot dimensions. A comprehensive analysis of the temperature dependence of the resonances points to protection from low-energy acoustic phonon scattering as the primary mechanism for linewidth narrowing. The latter underscores the effectiveness of lateral confinement as a method for engineering polariton-phonon interaction at high temperatures. This work thus establishes the feasibility of GaAs-based polariton structures with long temporal coherence at high temperatures.

## HL 20: 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, Doris Reiter, and Christoph Kastl)

Time: Tuesday 9:30–12:15 Location: EW 203

**Invited Talk** HL 20.1 Tue 9:30 EW 203

**Coherent ultrafast exciton dynamics mediated by vibronic couplings** — •Antonietta De Sio — Universität Oldenburg

The ultrafast dynamics of non-equilibrium excitations in functional materials and nanostructures, triggered by light-matter interaction, rely on a complex interplay between electronic and nuclear motion. Vibronic couplings may significantly influence the initial energy flow and charge motion following photoexcitation. In-depth understanding of the underlying physics of photoinduced ultrafast phenomena is thus crucial for steering nanoscale energy and charge transport, for the rationale design of efficient new materials and development of quantum technologies. Most of the mechanisms underlying these processes occur on only few 100s-fs timescales, thus demanding methods combining high time resolution and the ability to unravel couplings. Here I would like to give an overview of our most recent results showing how two-dimensional electronic spectroscopy with <10 fs time resolution provides detailed new insight into the ultrafast coherent exciton dynamics in technologically relevant materials, spanning from organic semiconductors to perovskites, and the fundamental role of vibronic couplings in these dynamics[1-2]. Specifically, we recently discovered intermolecular conical intersections in thin films of quadrupolar dyes governing ultrafast energy relaxation within <50 fs. In halide perovskites, we recently unveiled exciton Rabi oscillations driven by coherent phonon fields. Our results also suggest strategies to control ultrafast coherent dynamics in functional materials. [1] De Sio et al, Nature Nano. 16, 63 (2021) [2] Nguyen et al, Nature Comm. 14, 1047 (2023)

**Invited Talk** HL 20.2 Tue 10:00 EW 203

**Merging electron microscopy with advanced photonics** — •Armin Feist[1,2], Guanhao Huang[3,4], Germaine Arend[1,2], Yujia Yang[3,4], Jan-Wilke Henke[1,2], Arslan Sajid Raja[3,4], F. Jasmin Kappert[1,2], Rui Ning Wang[3,4], Hugo Lourenço-Martins[1,2], Qiu Zheru[3,4], Junqiu Liu[1,2], Ofer Kfir[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

Introducing light optics in state-of-the-art electron microscopes enabled quantum-coherent electron-light interaction [1] and the study of ultrafast nanoscale processes using coherent electron pulses [2]. Recently, high-$Q$ integrated photonics extended these capabilities to continuous electron beams for $\mu$eV-resolved electron spectroscopy [3].

Here, we show the coupling of single electrons and photons at a high-$Q$ integrated photonic microresonator [4]. Spontaneous scattering at empty resonator modes creates electron-photon pair states [5], enabling single-particle heralding schemes and noise-suppressed mode imaging. This provides a pathway towards novel hybrid quantum technology with entangled electrons and photons as well as electron-probing with tailored sensitivity for specific material excitations.

[1] A. Feist *et al.*, Nature **521**, 200 (2015). [2] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017). [3] J.-W. Henke *et al.*, Nature **600**, 653 (2021). [4] A. Feist *et al.*, Science. **377**, 777 (2022). [5] X. Bendaña *et al.*, Nano Lett. **11**, 5099 (2011).

**Invited Talk** HL 20.3 Tue 10:30 EW 203

**Nanotextured Surfaces Based on DNA** — •Irina Martynenko and Tim Liedl — Ludwig Maximilian University of Munich (LMU), Department Physics, Geschwister-Scholl-Platz 1, 80539 Munich, Germany

A longstanding goal of material scientists is to fabricate functional materials in which nanoscale objects are precisely positioned on macroscale surfaces. This can be achieved by a combination of bottom-up techniques, such as molecular self-assembly of DNA origami, and top-down lithographic methods. Through DNA origami placement (DOP) on lithographically patterned surfaces a variety of nanoscale components such as organic dyes, proteins or nanoparticles, have already been patterned on large-scale arrays [1, 2]. However, any DOP methods developed so far were limited to two-dimensional DNA origami structures and thus resulted in flat patterns and arrays only. Here we extend DOP to the third dimension through positioning of three-dimensional DNA origami onto nanometer-precise patterns over micro- and even millimeter scales [3]. We demonstrate that our method can produce surfaces nanotextured with three-dimensional hybrid DNA-silica structures with controllable heights up to 50 nm and a feature size down to ~ 6 nm. We believe that the presented strategy can be used for the assembly of a wide range of materials from metals and semiconductors to functional biomolecules arranged in virtually any three-dimensional geometry on large-scale substrates.

[1] R. Kershner, Nat Nanotechnol (2009) [2] A. Gopinath, et al., Nature (2016) [3] I. Martynenko et al., Nat Nanotechnol (2023)

**15 min. break**

**Invited Talk** HL 20.4 Tue 11:15 EW 203

**Advances in Quantum Light Generation for Quantum Communication** — •Tobias Heindel — Institute for Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany

In this contribution, I will review advances in the generation of flying qubits from solid-state quantum emitters for implementations of quantum communication and networking [1,2]. One spotlight will be on the progress in the on-demand generation of single indistinguishable photons in the telecom C-band exploiting pulsed coherent pumping schemes. Prospects for further improvements are discussed. Moreover, the development of plug-&-play benchtop single-photon quantum key distribution (QKD) systems as well as the transfer to emerging quantum emitter platforms (e.g. 2D quantum materials) are highlighted. Not least, recent experiments towards the generation of multi-partite entangled states are presented, thereby building the bridge from fundamental quantum optics to applications in quantum information.

Many people contributed to this work, including my team members D. A. Vajner, L. Rickert, T. Gao, K. Kaymazlar, N. Kewitz, and M. von Helversen as well as the members of collaborating groups - I express my gratitude to all of them. Financial support by the German Federal Ministry of Education and Research (BMBF) via the Quantum Futur grant "QuSecure" and the BMBF joint project "tubLAN Q.0" as well as by the Einstein Foundation via the Einstein Research Unit "Quantum Devices" is acknowledged.

[1] Vajner et al., Advanced Quantum Technologies 5, 2100116 (2022) [2] Heindel et al., Advances in Optics and Photonics 15, 613 (2023)

**Invited Talk** HL 20.5 Tue 11:45 EW 203

**Membrane external-cavity surface-emitting lasers: A review at the first decade of research** — •Hermann Kahle — Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP), and Department of Physics, Paderborn University, 33098 Paderborn, Germany

Membrane external-cavity surface-emitting lasers (MECSELs) have emerged as a derivative of vertical-external-cavity surface-emitting lasers (VECSELs). The pursuit of higher output power, particularly in materials with moderate performance characteristics, has driven the innovation of creating extremely thin amplifier membranes within a nearly ideal thermal environment. These gain membranes, sandwiched between transparent heat spreaders, containing nothing else but the active region of a VECSEL (no substrate, no monolithically integrated DBR), caught much attention in recent years. Inserting the gain element into a cavity completes the MECSEL, which has already enabled access to laser wavelengths previously unattainable by VECSELs and has facilitated watt-level output power at room temperature. Furthermore, the MECSEL approach fundamentally enables the production of high-power lasers of the highest beam quality whenever it is possible to produce an LED. Beyond that, the membrane approach offers numerous additional advantages.

A comprehensive discussion of these advantages will be provided, as well as a review of the developments that have contributed to the success of MECSELs. The conclusion will give an overview of the most recent findings and a glimpse into future developments in this field.

## HL 21: Heterostructures, Interfaces and Surfaces I

Time: Tuesday 9:30–11:45 Location: EW 561

HL 21.1 Tue 9:30 EW 561

**Surface passivation and detrimental heat-induced diffusion effects in RbF-treated Cu(In,Ga)$Se_2$ solar cell absorbers** — •Amala Elizabeth[1], Sudhir K. Sahoo[2], Tim Kodalle[3], Thomas D. Kühne[2], Christian A. Kaufmann[3], Hossein Mirhosseini[2], and Harry Mönig[1] — [1]University of Münster, Münster, Germany — [2]University of Paderborn, Paderborn, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Recent efficiency gains by Cu(In,Ga)$Se_2$ (CIGS)-based thin film solar cells (> 23%) are largely attributed to post-deposition treatments (PDTs) using alkali metal compounds like RbF and CsF. Consequently, comprehending the impact of alkali PDTs on the electronic defect physics of these absorber surfaces is crucial for understanding p/n junction formation and further device optimization.

Here we present a combined analytical study of the RbF-CIGS surface using scanning tunneling spectroscopy (STS) and X-ray photoelectron spectroscopy (XPS). STS results reveal the effectiveness of RbF PDT in preventing surface oxidation and consequently passivating electronic defect levels at the absorber surface. Ab-initio density functional theory (DFT) calculations corroborate this passivating effect. However, heat treatment at temperatures as low as 100°C was found to induce Rb diffusion, leading to increased electronic defect levels at the surface and potential deterioration of the p/n-junction interface. This study emphasizes the dual impact of RbF PDT, with its advantages and potential drawbacks, especially during subsequent device fabrication steps at elevated temperatures.

HL 21.2 Tue 9:45 EW 561

**Depth profiling of defects with nanometer resolution at semiconductor interfaces using low-energy muons** — •Thomas Prokscha[1], Maria Martins[1,2], Piyush Kumar[2], Marianne Bathen[2], Xiaojie Ni[1], Judith Wörle[2], and Ulrike Grossner[2] — [1]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [2]Advanced Power Semiconductor Laboratory, ETH Zurich, 8092 Zurich, Switzerland

Defects and structural changes at semiconductor interfaces are of fundamental importance for the performance of semiconductor devices. While a variety of characterization methods exists for the investigation of process-induced defects, most of these techniques cannot resolve the depth distribution of defects close to the interfaces, an information which is important to better understand the relation between these defects and the observed limitations in device performance. Here we use low-energy muon spin spectroscopy as a powerful tool to study the distribution of defects in semiconductors with unprecedented nanometer depth resolution. The technique is based on studying the effect of defects on the formation probability of hydrogen-like muonium states in semiconductors and semiconductor-oxide interfaces. We used proton irradiated Si and 4H-SiC to measure the effect of well-defined defect concentrations profiles on the formation of muonium states, and apply this new technique to the study of technologically relevant SiO2/Si and SiO2/SiC interfaces [1,2].

[1] M. Martins et al., Adv. Mat. Inter. 10, 2300209 (2023).
[2] P. Kumar et al., Phys. Rev. Appl. 19, 054025 (2023).

HL 21.3 Tue 10:00 EW 561

**Investigation Of Dielectric Parameters Of ZnO/p-Si Diode**

**At Room Temperature** — •Ali Orkun Çağirtekin, Ahmad Ajjaq, Özlem Barin, Pinar Oruç, and Selim Acar — Department of Physics, Faculty of Science, Gazi University, Ankara, Turkey

In this study; ZnO/p-Si nanostructure was obtained with a two-step process. First, a ZnO nucleating layer was produced on p-type silicon substrate by the dip coating method. Then, the core-coated sample was exposed to a 95 * and 3-hour hydrothermal reaction and the production of ZnO nanostructures was achieved. Finally, silver contact was applied to the produced structure by thermal evaporation. SEM analysis results show that ZnO nanostructures are coated homogeneously on the silicon substrate without gaps. It was aimed to investigate the performance properties of the produced diode under different conditions for different applications. Current-voltage, capacitance-frequency and conductance-frequency measurements of the ZnO/p-Si diode were measured at room temperature between 2 kHz and 1 MHz. As a result of these measurements, the obtained diode displays a rectification of about seven orders of magnitude at a bias voltage of 4 V. The dielectric constant of the diode at 2 kHz at room temperature was calculated as 13, dielectric loss as 10, and dielectric loss tangent as 0.79. It was also observed that there was a peak in the imaginary part of the electrical modulus. Finally, in the conductivity parameter, it was observed that the conductivity increased as the frequency increased. According to the results obtained, it was seen that the ZnO surface layer was suitable for capacitor applications.

HL 21.4 Tue 10:15 EW 561

**Realization of the Topological Pseudospin-Hall Effect in an Exciton-Polariton Elliptical Micropillar Chain** — •Simon Widmann, Jonas Bellmann, Johannes Düreth, Siddhartha Dam, Christian G. Mayer, Philipp Gagel, Simon Betzold, Monika Emmerling, Sven Höfling, and Sebastian Klembt — Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik

We realize the topological pseudospin-Hall effect in a chain of elliptical exciton-polariton micropillars, using the different circular polarizations $\sigma_{\pm}$ as a pseudospin [1]. Elliptical micropillars are fabricated by fully etching a GaAs microcavity, creating a large confinement potential. The ellipticity of the micropillars leads to a linear polarization splitting along the semi-minor and major axis of the individual elliptical micropillars. In combination with a suitable placement into a lattice, this produces a system in which positive and negative momentum states have opposing circular polarizations. This experimental demonstration is a step towards the realization of the non-Hermitian skin effect in a chain of coupled elliptical micropillars.

[1] S. Mandal et al., ACS Photonics 9, 527-539 (2022)

**15 min. break**

HL 21.5 Tue 10:45 EW 561

**Effectiveness of an AlSb dislocation filter layer in the epitaxy of GaSb on Si(001)** — •Karl Graser[1], Audrey Gilbert[2], Steffen Richter[1], Jean-Baptiste Rodriguez[2], Eric Tournié[2], and Achim Trampert[1] — [1]Paul-Drude Institut für Festkörperelektronik, Leibnitz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Institut d'Electronique et des Systèmes , University of Montpellier, CNRS, F- 34000, France

The direct epitaxial growth of III-V semiconductors on Si (001) opens the door to the integration of III-V-based photonic devices with Si integrated circuits. Especially for the epitaxial growth of GaSb on Si with its high lattice mismatch, methods must be found to reduce the resulting huge number of threading dislocations which negatively affect the device performance. In the present study, the impact of a strained AlSb filter layer on the dislocation reduction for GaSb-on-Si epitaxy is investigated by transmission electron microscopy techniques. The site-specific measurements of dislocation density at different positions along the growth direction are used to calculate the filter efficiency, which is clearly related to the formation of misfit dislocation networks at the interfaces between AlSb and GaSb. It is shown that the nature of the dislocation networks, their line directions and Burgers vectors, is governed by epitaxial strain relief and complex dislocation reactions in the interfaces, and finally determines the effectiveness of threading dislocation reduction process.

HL 21.6 Tue 11:00 EW 561

**Implementation of polaritonic lattices using patterning and oversputtering techniques** — •David Laibacher, Johannes Düreth, Simon Betzold, Siddhartha Dam, Monika Emmerling, Sven Höfling, and Sebastian Klembt — Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg, Deutschland

Exciton-Polaritons have been a focus of study during recent years due to their ability to form a driven-dissppative Bose-Einstein-Condensate in two dimensions at finite temperatures. One way to study them accesibly is using a laser to generate exitons in an active material located between two distributed Bragg reflectors (DBR), confining the photon in one direction. In this work, the polaritonic potential landscape is manipulated due to confinement of it's photonic part by manipulating the length of the cavity layer in order to create different structures with components in the order of microns. The length of the cavity is manipulated by either etching a few tens of nanometers into (Etch and Oversputter) or depositing a similar thickness of $TiO_2$ discs onto (Deposition and Oversputter) the cavity layer. This enables the creation of polariton lattices with features in the order of nanometers, which was not possible using previously established techniques such as etching micropillars. The top DBR is deposited using sputtering, aiming to achieve a similar quality when compared to growing it using molecular beam epitaxy, thus allowing easier sample-generation and faster structural optimization.

HL 21.7 Tue 11:15 EW 561

**Realization of Higher Order Topological Insulators in Hybrid Dielectric-Semiconductor Microcavities** — •Johannes Düreth, Philipp Gagel, Simon Betzold, Siddhartha Dam, Christian G. Mayer, David Laibacher, Monika Emmerling, Sven Höfling, and Sebastian Klembt — Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Since its introduction to the polariton community by El Daïf and coworkers in 2006 [1], the etch-and-overgrowth method has been a very versatile technique for the generation of photonic confinement. It is perfectly suited to manufacture large, uniform and complex potential landscapes since the confinement as well as its coupling can be finely tuned by controlling the etch-depth. Here, we improve on this method by using a dielectric top mirror consisting of $SiO_2/TiO_2$ layers instead of an epitaxially grown one. In recent years, topological photonics has emerged as a powerful tool to engineer traits of optoelectronic applications. We implement 0-dimensional higher order topological defects in a *breathing* Kagome lattice, as well as a 2-D Su-Schrieffer-Heeger (SSH) lattice. Additionally, we show polariton lasing from the corner defect of the breathing Kagome lattice and the 0-D defect of the 2D-SSH lattice, as well as their coherence properties [2].

[1] O. El Daïf et al., Appl. Phys. Lett. 88, 061105 (2006)
[2] P. Gagel, J. Düreth et al., in preparation (2023)

HL 21.8 Tue 11:30 EW 561

**Chemical and energetical structure at P-rich InP(100)/$TiO_2$ heterointerface** — •Agnieszka Paszuk[1], Jennifer Velázquez Rojas[2], Mohammad Amin Zare Pour[1], David Ostheimer[1], Christian Höhn[2], Roel van de Krol[2], and Thomas Hannappel[1] — [1]Fundamentals of Energy Materials, Technische Universität Ilmenau — [2]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

In the photoelectrochemical cells with the highest solar-to-hydrogen conversion efficiencies, III−V photoabsorbers are integrated with a metal oxide passivation layer and a catalyst. Such devices require preparation of ideal (buried)interfaces to minimize the losses of the photogenerated charge carriers. Here, we study atomic layer deposition (ALD) of $TiO_2$ on phosphorus terminated (P-rich) InP(100) surfaces prepared in a metalorganic vapor phase epitaxy reactor. Samples were transferred in ultra-high vacuum to an ALD chamber. Titanium tetrachloride and water were used as the titanium and oxygen precursors, respectively. The preparation of P-rich InP(100) and the deposition of the $TiO_2$ were monitored *in situ* by ellipsometry and optical spectroscopy, respectively. After selected precursor pulses, the surface chemical composition and the electronic structure were determined by photoemission spectroscopy. We observed a nucleation delay of $TiO_2$ and during the first deposition cycles, a limited interaction of the water and the Ti precursor due to stable P-P bonds on the InP(100) surface.

The $TiO_2$ layers show +4 oxidation state and we find no evidence of the presence of $Ti^{3+}$ state, which might act as trap centres.

## HL 22: Focus Session: Young Semiconductor Forum

This poster session is part of the Young Semiconductor Forum, which is a platform for post-docs at all career stages to present themselves and their scientific ideas. The forum 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 AGYouLEAP (Susanne Liese, Alexander Schlaich, Doris Reiter und Christoph Kastl).

Time: Tuesday 11:00–15:30 Location: Poster F

HL 22.1 Tue 11:00 Poster F

**High-entropy thermoelectrics: what is the role of metavalent bonding?** — •Nan Lin[1], Dongwang Yang[2], Yuan Yu[1], and Matthias Wuttig[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China

The design principle of high-entropy (HE) thermoelectrics is still elusive because forming a solid solution is the prerequisite to enhance the configurational entropy. Typical HE thermoelectrics have been mainly realized in chalcogenides such as PbTe and GeTe, etc. Interestingly, these chalcogenides also show an unconventional chemical bonding mechanism, termed metavalent bonding (MVB). Is there a strong coincidence of correlation between HE thermoelectrics and MVB? To answer this question, we designed PbQ-AgBiQ2 (Q = S, Se, Te) samples to study their microstructures and bonding mechanisms, as well as thermoelectric properties. We observe no obvious phase separations in these alloys. Atom probe tomography measurements also confirm the abnormal bond-breaking behavior, corroborating their bonding mechanism. Moreover, the maximum optical absorption decreases from Q = Te to Q = Se and then to Q=S due to the increased charge transfer. This also leads to the weakening of MVB. The thermoelectric properties decrease with increasing the charge transfer numbers from tellurides to sulfides. This work indicates that mixing metavalently bonded solids with a controlled degree of charge transfer could be an important avenue for designing HE thermoelectrics.

HL 22.2 Tue 11:00 Poster F

**Shaped pulses for quantum dots- Innovations and future perspectives** — •Vikas Remesh — Institute for Experimental Physics, University of Innsbruck, Technikerstr. 25d, 6020 Innsbruck, Austria

Shaped laser pulses have been remarkably effective in investigating and controlling various light-matter interactions spanning a broad area of research from laser technology to nanophotonics. In quantum technology, the pulse shaping techniques to generate complex spatiotemporal waveforms have found renewed interest, for instance in coherent control of quantum dots, spectrotemporal mode shaping for parametric down conversion source and so on. In this talk, I will navigate through the impact of pulse shaping techniques in nanospectroscopy and how it enabled us to demonstrate efficient preparation schemes in quantum dots, highlighting our recent works [1-4]. Afterwards, I will conclude with my vision on the future of nanophotonics-assisted-quantum technologies. [1] ACS Photonics 6, 2487 (2019), ACS sensors 6, 581 (2021) [2] Nano Letters 22, 6567 (2022) [3] Materials for Quantum Technology 3, 025006 (2023) [4] APL Photonics 8, 101301 (2023), arXiv:2305.20017

HL 22.3 Tue 11:00 Poster F

**Membrane external-cavity surface-emitting lasers: A review at the first decade of research** — •Hermann Kahle — Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP) and Department of Physics, Paderborn University, 33098 Paderborn, Germany

Membrane external-cavity surface-emitting lasers (MECSELs) have emerged as a derivative of vertical-external-cavity surface-emitting lasers (VECSELs). The pursuit of higher output power, particularly in materials with moderate performance characteristics, has driven the innovation of creating extremely thin amplifier membranes within a nearly ideal thermal environment. These gain membranes, sandwiched between transparent heat spreaders, containing nothing else but the active region of a VECSEL (no substrate, no monolithically integrated DBR), caught much attention in recent years. Inserting the gain element into a cavity completes the MECSEL, which has already enabled access to laser wavelengths previously unattainable by VECSELs and has facilitated watt-level output power at room temperature. Furthermore, the MECSEL approach fundamentally enables the production of high-power lasers of the highest beam quality whenever it is possible to produce an LED. Beyond that, the membrane approach offers numerous additional advantages.

A comprehensive discussion of these advantages will be provided, as well as a review of the developments that have contributed to the success of MECSELs. The conclusion will give an overview of the most recent findings and a glimpse into future developments in this field.

HL 22.4 Tue 11:00 Poster F

**Tunable White-Light Emission from Self-Trapped Excitons in Low-Dimensional Hybrid Perovskites** — •Philip Klement[1], Lukas Gümbel[1], Johanna Heine[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Department of Chemistry, Universität Marburg, Germany

Lead halide perovskites and related main group metal halide materials hold immensie potential for advanced solar cells and LEDs. Efficient light emission in these materials relies on self-trapped excitons, where excitations create temporary defects that trap excitons within the crystal lattice. However, the complex interplay of factors like ground- and excited-state distortions, lattice softness, and electron-phonon coupling hinders designing these materials for specific optical properties. Here, we study various antimony and bismuth halide compounds with systematic variations in composition, anion dimensionality, connectivity, and chiral organic cation. The unique crystal structure of these compounds facilitates the formation of self-trapped excitons, resulting in broad photoluminescence emission with large Stokes shifts, which we correlate with structural parameters. Challenging conventional wisdom, we present single layers of a 1D hybrid perovskite, questioning the belief that atomically thin 2D materials require in-plane covalent bonding. The thickness-dependent exciton self-trapping induces a pronounced shift in emission energy, revealing distinctive exciton physics. Furthermore, we investigate charge carrier diffusion using temporally and spatially resolved photoluminescence spectroscopy. Our findings deepen the comprehension of emission processes in hybrid materials.

HL 22.5 Tue 11:00 Poster F

**Doping-control of excitons and magnetism in few-layer CrSBr** — •Farsane Tabataba-Vakili[1,2], Huy Nguyen[1], Anna Rupp[1], Kseniia Mosina[3], Anastasios Papavasileiou[3], Patrick Maletinsky[4], Mikhail Glazov[5], Zdenek Sofer[3], Anvar Baimuratov[1], and Alexander Högele[1,2] — [1]Fakultät für Physik, Munich Quantum Center, and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, München, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic — [4]Department of Physics, University of Basel, Basel, Switzerland — [5]Saint Petersburg, Russia

In 2D magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-

layer CrI3. Air-stable CrSBr stands out as an antiferromagnetic semiconductor with excitons coupled to the magnetic order and exciton-magnon coupling. I will present our work on doping-control of excitons and magnetism in few-layer CrSBr. 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.

HL 22.6 Tue 11:00 Poster F

**Straintronics with van der Waals materials** — •Emeline Nysten — Physikalisches Institut, Universität Münster, Germany

Surface acoustic waves (SAWs) have proven to be a multifaceted and efficient tool for the control of semiconductor nanostructures optical properties and the dynamical transport of charge carriers [1]. By integrating 2D semiconducting transition metal dichalcogenides (TMDCs) onto SAW-devices, we are able to investigate and control their interesting optoelectronic properties. Firstly, by systematically studying the SAW-modulated emission of a $WSe_2$ monolayer in the time domain, we unravel the impact of ubiquitous inhomogeneities in 2D TMDCs on charge carrier dynamics, outperforming conventional static photoluminescence measurements. Secondly, the study of the photogated SAW-induced acousto-electric effect in $WSe_2$ provides detailed insight into the underlying charge carrier dynamics and the nature of the contact between electrode and 2D semiconductor. Finally, I will discuss perspectives to employ SAW to selectively manipulate emergent phenomena like interfacial ferroelectricity and exciton dynamics in van der Waals heterostructures. [1] Delsing et al., "The 2019 surface acoustic waves roadmap" J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 22.7 Tue 11:00 Poster F

**Elucidating the mechanism of spectral diffusion in colloidal quantum dots** — Frieder Conradt, Vincent Bezold, Volker Wiechert, Steffen Huber, Stefan Mecking, Alfred Leitenstorfer, and •Ron Tenne — University of Konstanz, Konstanz, Germany

Thanks to their exceptional tunability and ease of integration into semiconductor-based devices, colloidal quantum dots (CQDs) have found widespread technological implementations such as display technology. To expand this success into quantum applications, spectral stability and coherence, two closely linked topics, need to be addressed. I will describe recent efforts in answering two fundamental questions: what are the time scales of spectral fluctuations in the emission of a CQD and what is their underlying cause? We perform high-resolution photoluminescence spectroscopy of single particles at low temperatures as a function of an applied electric bias. Doing so, we provide the first direct evidence that spectral fluctuations are straightforwardly derived from the sensitivity of the emission spectrum to spurious electric fields, thus identifying the quantum-confined Stark effect as their physical mechanism.

HL 22.8 Tue 11:00 Poster F

**Guided light in Angstrom thin samples - 2D van der Waals materials as a platform for novel optical devices and fundamental research** — •Patryk Kusch, Mira Kressler, and Stephanie Reich — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Van der Waals materials, like graphene and transition metal dichalcogenides (TMDCs), offer exciting physical properties to explore such as high charge mobility, mechanical strength, and strong light emission. Particularly, monolayers of TMDCs are direct semiconductors that exhibit strong optical absorption by tightly bound excitons, quasiparticles formed by a bound state of an electron, and a hole within one monolayer. The binding energy is often so strong (several 100 meV) that they can be excited under ambient conditions. Furthermore, TMDCs promote the waveguiding of light. As we showed waveguided modes can propagate over several tens of micrometers through a 60 nm thin slab of $MoS_2$, which is interesting for the realization of novel optical devices. Here we demonstrate that light can be guided in Ångstrom thin $WS_2$ by imaging waveguided modes in real space with the scattering type scanning near-field optical microscope. The guided light couples with excitons, leading to the formation of exciton-polaritons, quasi-particles that are currently the focus of many scientific studies. We get access to their dispersion relation by taking nanoimages of the propagating polaritons at different excitation energies around the A and B exciton. It impressively shows that the coupling strength between guided light and excitons is in the strong coupling regime.

HL 22.9 Tue 11:00 Poster F

**Electrolytes at semi-conducting materials: From first principles to coarse-grained models** — •Alexander Schlaich — SC SimTech, University of Stuttgart

The structure and dynamics of liquid electrolytes at semi-conducting materials is fundamental for applications ranging from energy storage via electrocatalysis to functional and responsive materials. However, modeling such systems is intricate since electrostatic interactions * and possibly charge transport * require to consider quantum-mechanical effects, whereas structural re-arrangements, charge transport and slow dynamics demand for long time- and length-scales. In this contribution I will summarize the work in my group showing how first-principle information can be incorporated to semi-classical molecular models to cover relevant scales. We further develop based on this information continuum models to target application-scale problems, i.e., bridge to full range from the micro- to the macro-scale. I will give an outlook showing examples from CO2-reduction in confined systems to coupled ionic-electronic transport in systems of conjugated polymers. I will also elaborate on our efforts making the corresponding workflows F.A.I.R. (findable, accessible, interoperable and reusable) by strict documentation and especially by including also the analysis of data, which too often is still neglected in discussions about scientific software.

HL 22.10 Tue 11:00 Poster F

**Route toward simulating semiconductor interfaces and surfaces: from crafting an XC potential to applications** — •Tomáš Rauch — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Since 2018 I have been part of the project "Developing an e-lab for interfaces on demand – dandelion" funded by the VW Foundation. My work toward describing structural and electronic properties of inhomogeneous systems with ab initio methods consisted of several steps which I will present in my talk. First, having to describe heterostructures with large supercells using DFT, I crafted [1], implemented, and benchmarked [2] a new XC potential suitable for the particular problem. Further, finding the commonly used concept of projected DOS not sufficient for strongly reconstructed interfaces or surfaces, I developed a program to calculate local DOS from the output of the VASP code [3]. Finally, I will present my results for specific cases, including CdTe shells on InSb, thin $SrTiO_3$ covering Si, and surfaces of CuI [4].

[1] T. Rauch *et al.*, J. Chem. Theory Comput. **16**, 2654 (2020).

[2] T. Rauch *et al.*, Phys. Rev. B **101**, 245163 (2020); T. Rauch *et al.*, J. Chem. Theory Comput. 17, 4746 (2021); A. Ghosh *et al.*, J. Chem. Phys. **157**, 124108 (2022).

[3] L. Lodeiro and T. Rauch, Comp. Phys. Commun. **277**, 108384 (2022)

[4] G. Badawy *et al.*, Adv. Sci. **9**, 2105722 (2022); T. Rauch *et al.*, Phys. Rev. B **107**, 115303 (2023)

HL 22.11 Tue 11:00 Poster F

**Exciton-exciton interactions in van der Waals heterobilayers** — •Alexander Steinhoff[1], Edith Wietek[2], Matthias Florian[3], Tommy Schulz[1], Takashi Taniguchi[4], Kenji Watanabe[4], Shen Zhao[5], Alexander Högele[5], Frank Jahnke[1], and Alexey Chernikov[2] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]Institute of Applied Physics, Technische Universität Dresden, Germany — [3]University of Michigan, Department of Electrical Engineering and Computer Science, Ann Arbor, USA — [4]National Institute for Materials Science, Tsukuba, Japan — [5]Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany

Exciton-exciton interactions are key to understanding non-linear optical and transport phenomena in van der Waals heterobilayers, which emerged as versatile platforms to study correlated electronic states.

We present a combined theory-experiment study of excitonic many-body effects based on first-principle band structures and Coulomb interaction matrix elements. We demonstrate that dipolar blue shifts are almost perfectly compensated by many-body effects, mainly by screening-induced self-energy corrections. Moreover, we identify a crossover between attractive and repulsive behavior at elevated exciton densities.

Our results revise the established picture of dipolar repulsion dominating exciton-exciton interactions in van der Waals heterostructures and open up opportunities for their external design.

HL 22.12 Tue 11:00 Poster F

**Non-Hermitian Physics in multiterminal devices** — Kyryl Ochkan[1], Viktor Könye[1], Louis Veyrat[1], Anastasiia Chyzhykova[1], Romain Giraud[1], Dominique Mailly[2], Antonella Cavanna[2], Ulf Gennser[2], Ewelina Hankiewicz[1], Bernd Büchner[1], Jeroen Van den Brink[1], Jan Carl Budich[1], Ion Cosma Fulga[1], and •Joseph Dufouleur[1] — [1]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany — [2]Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Saclay, Palaiseau, France

One of the simplest examples of non-Hermitian topology is encountered in the Hatano-Nelson (HN) model, a one-dimensional chain where the hopping in one direction is larger than in the opposite direction. We present here the first experimental observation of non-Hermitian topology in a quantum condensed-matter system made of a multi-terminal quantum Hall device etched in a high mobility GaAs/AlGaAs two-dimensional electron gas ring. In our device, we directly measure and evidence the non-Hermitian skin effect. We also compute for our experimental device two topological invariants that are found to be more robust than the Chern number. We finally use the unique properties of our system and continuously tune the system configuration between open and periodic boundary conditions [1]. We also present the latest developments with regard to the application to electronic devices that can be used as topological ohmmeters [2].

[1] K. Ochkan et al. (arXiv:2305.18674, Nature Physics - in press) [2] V. Könye, et al. (arXiv:2308.11367, under review)

HL 22.13 Tue 11:00 Poster F

**Where physics meets biology** — •Susanne Liese — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Augsburg, Germany

All biological processes are governed by physical principles. A fundamental understanding of biological functionality therefore requires an in-depth understanding of the underlying biophysical mechanisms. Using mathematical and numerical modeling, we can explore questions at the intersection between physics, biology, and chemistry. These studies include diverse aspects such as the binding dynamics of multivalent pathogen-inhibitor interactions and the intricate formation and interactions within both membrane-bound and membraneless organelles. In this presentation, I will present how these models serve as a key to deciphering the underlying action and organizational principles that drive the formation and self-organization of biological and soft matter systems.

HL 22.14 Tue 11:00 Poster F

**Efficient Narrow-Beam Hexagonal Boron-Nitride Single-Photon Source** — •Johann A. Preuss[1], Helge Gehring[1,2], Robert Schmidt[1], Lin Jin[1,2], Daniel Wendland[1,2], Johannes Kern[1], Wolfram H.P. Pernice[1,2,3], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]University of Münster, Institute of Physics and Center for Nanotechnology, 48149 Münster, Germany — [2]University of Münster, Center for Soft Nanoscience, 48149 Münster, Germany — [3]Kirchhoff-Institute for Physics, University of Heidelberg, 69120 Heidelberg, Germany

Robust quantum light sources are important for creating quantum networks. Hexagonal boron nitride (hBN) and other 2D materials host single-photon emitters that offer bright emission, even at room temperature, rendering them promising for quantum applications. However, efficient photon collection is difficult due to their wide-angled emission pattern. To enhance light collection, we 3D-printed polymer microlenses onto individual hBN nanocrystals, to collimate single-photon emission into a low-divergent beam. Photoluminescence and photon correlation measurements demonstrate that our ultra-low fluorescence photoresin does not alter the spectrum of the emitters and preserves the single-photon character of the emitted light. Importantly, by analyzing the emission pattern, we show that the lenses efficiently collimate the emission to angles below 5°, enabling the use of collection lenses with low numerical apertures or direct coupling into optical fibers.

HL 22.15 Tue 11:00 Poster F

**Field-induced hybridization of moiré excitons** — •Anvar Baimuratov — Fakultät für Physik, Munich Quantum Center, and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München, Germany

We study experimentally and theoretically the hybridization among intralayer and interlayer moiré excitons in a MoSe2/WS2 heterostructure. Using a dual-gate device and cryogenic white light reflectance and narrow-band laser modulation spectroscopy, we subject the moiré excitons in the MoSe2/WS2 heterostack to a perpendicular electric field, monitor the field induced dispersion and hybridization of intralayer and interlayer moiré exciton states, and induce a cross-over from type I to type II band alignment. Moreover, we employ perpendicular magnetic fields to map out the dependence of the corresponding exciton Landé g-factors on the electric field. Finally, we develop an effective theoretical model combining resonant and non-resonant contributions to moiré potentials to explain the observed phenomenology, and highlight the relevance of interlayer coupling for structures with close energetic band alignment as in MoSe2/WS2.

HL 22.16 Tue 11:00 Poster F

**Nonlinear dynamics: from machine tools to nanoresonators** — •Ahmed A. Barakat and Eva M. Weig — Technical University of Munich, Munich, Germany

Exactly as stated by Nikola Tesla: "If you wish to understand the universe, think of energy, frequency, and vibration", this was the repeatedly proven conclusion through studying machine tools, wind turbines, microgyroscopes, microwave cavities and quantum systems. The theory of nonlinear dynamics has always been essential to accurately analyze oscillations since most physical processes are inherently nonlinear, however, allowing linearization under tight conditions. This mere fact was the primary motivation to delve into nonlinear dynamics after observing self-oscillations in lathes and aeroelastic wings. The focus, afterwards, was studying one of the most common nonlinear mathematical descriptions in micro and nanosystems, those combining the ubiquitous cubic nonlinearities and parametric effects in multi-modal systems, forming the so-called Mathieu-Duffing systems. This theoretical study was exploited to explain the oscillatory behavior of microgyroscopes. Recently, this study has been extended to studying the modal coupling in nanomechnical string resonators, which showed a similar behavior under parametric excitation. Most interestingly is exploiting the parametric normal mode splitting phenomenon to study the coupling strength between both modes, which would be a novel approach that could be generalized to other two-mode, or two-level, systems.

HL 22.17 Tue 11:00 Poster F

**Towards SiC as a Platform for Hybrid Quantum Technologies** — •Philipp Bredol, Felix David, and Eva Weig — Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

Established nano electronic devices rely mostly on classical physics. Quantum effects offer to go beyond the possibilities of classical devices, but are difficult to exploit due to their fragile nature. Hybrid devices aim to combine the advantages of both worlds by combining quantum and classical elements. However, integration on a single hybrid chip is a challenging task, because materials and process chemistry have to be compatible.

Silicon carbide (SiC) is an exceptional material that is feasible for both classical and quantum electronics: Classical transistors are already being fabricated from SiC on an industrial scale for power electronics. At the same time, SiC hosts color centers with lifetimes competitive with the nitrogen-vacancy center in diamond, which makes it interesting for quantum sensing and quantum information applications. Last but not least, SiC is well suited for high-$Q$ nanomechanics, which can mediate couplings between degrees of freedom that only weakly couple in a direct manner. We explore the possibilities of SiC based hybrid quantum technologies from the nanomechanical perspective. As a first step, we compare the nanomechanical properties of devices fabricated from the 3C and 4H SiC polytypes using various fabrication methods.

HL 22.18 Tue 11:00 Poster F

**Broken symmetries in two-dimensional materials probed by nonlinear optoelectronic transport** — •Christoph Kastl — Walter Schottky Institute and Physik-Department, Technical University of Munich, Germany — Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

I will present examples of (un)intentionally broken symmetries in van der Waal materials and the resulting nonlinear optoelectronic transport. For $MoTe_2$, photocurrent imaging reveals a disordered transition between the monoclinic phase to the low-temperature orthorhombic phase, where ultrafast photocurrents originate from the local breaking

of the electronic symmetries (2D Mater. 2022, 9, 011002). In graphene-based circuits, we address gate-tunable, non-linear transport arising from strong spin-orbit coupling, which may be used to manipulate spin-polarized carriers by both optical and electrical means. In commensurate graphene/$Bi_2Te_2Se$ interfaces, we find an enhanced helicity-dependent photocurrent due to the peculiar spin-orbit proximity of the commensurate alignment (ACS Nano 2022, 16, 12338-12344). In graphene/$WTe_2$, we demonstrate optical detection of current-induced spin polarisations related to a nonlinear anomalous Hall effect in the heterostructure (Nat. Commun. 2022, 13, 3152). Finally, I will discuss recent work towards top-down control of electronic symmetries by nanofabricaton of lateral superlattice structures in van der Waals materials. The research is supported through the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No 101076915 (2DTopS).

HL 22.19 Tue 11:00 Poster F

**Ultrahigh frequency Brillouin spectroscopy in optophononic Fabry-Perot cavities and optomechanical study of 2D materials in fiber Fabry-Perot cavities** — •Anne Rodriguez — Chair for Nano and Quantum Sensors, Technische Universität München, Garching, Germany

The fine control achieved over acoustic phonon dynamics enabled the engineering of interactions with other excitations [1,2]. During my PhD thesis (C2N, CNRS, Université Paris-Saclay) my research was mainly focused on the study of acoustic phonons in GaAs/AlAs multilayered cavities where both light in the near-infrared range and acoustic phonons in the 20 GHz range can be simultaneously confined. I developed experimental approaches for Brillouin spectroscopy that can integrate a widely tunable excitation-source to probe ultra-high acoustic phonons [3,4]. My work also involved theoretical research on topological 1D phononic resonators [5]. In October 2023, I joined the Nano and Quantum Sensor group (TUM) where I am working on optomechanics with transition metal dichalcogenides membranes. I aim to study the mechanical properties and the strain coupling with a quantum emitter embedded in the membrane [6] in a fiber Fabry-Perot cavity. This would be a step forward in the study of spin-optomechanics [7].

[1]M. Yuan et al., AVS Quantum Sci. 4, 035901 (2022). [2]Y. Chu et al., Science 358, 199 (2017). [3]A. Rodriguez et al., Opt. Exp. 29, 2637 (2021). [4]A. Rodriguez et al., ACS Phot. 10, 1687 (2023). [5]A. Rodriguez et al., PRB 108, 205301 (2023). [6]K. Barthelmi et al., APL 117, 070501 (2020). [7]L. He et al., Sci. Adv. 2, e1600485 (2016).

HL 22.20 Tue 11:00 Poster F

**Ultrafast coherent control of single-photon emitters in hBN** — Johann A. Preuss[1], Daniel Groll[1], Robert Schmidt[1], Thilo Hahn[1], Pawel Machnikowski[2], Tilmann Kuhn[1], Daniel Wigger[3], and •Steffen Michaelis de Vasconcellos[1] — [1]Universität Münster, Germany — [2]Wrocław University of Science and Technology, Poland — [3]Trinity College Dublin, Ireland

Single-photon sources are essential building blocks for quantum networks, and their coherent control remains a key challenge. Recently, single-photon sources in 2D van der Waals materials joined the family of solid-state quantum light emitters. In hexagonal boron nitride (hBN), optically active states have been discovered that efficiently emit single photons even at room temperature. This emitter's variable emission wavelength, narrow lines, and tunability make it promising for quantum sensing and wavelength division multiplexed quantum communications. Our study demonstrates femtosecond coherent state manipulation of individual hBN quantum emitters, showcasing resonant and phonon-assisted control mechanisms. The joint experiment-theory study explores the effects of different sources of spectral jitter on the ultrafast coherence dynamics and how the dephasing of optical and acoustic phonons affects the coherence. Our experiments on phonon-assisted ultrafast coherent control of individual hBN color centers are an important step towards hybrid quantum technologies that combine electronic and phononic excitations.

## HL 23: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing I (joint session TT/DY/HL/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.
This joint session will be continued Wednesday afternoon (TT53) and Thursday morning (TT70). Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Tuesday 11:45–13:00 Location: H 3007

HL 23.1 Tue 11:45 H 3007

**Josephson Optomechanics** — •Surangana Sengupta[1], Bjoern Kubala[1,2], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]ICQ and IQST, Ulm University, Germany — [2]DLR-QT, German Aerospace Center, Ulm, Germany

In recent years, optomechanical cooling using microwave radiation has been realized in various superconducting circuits with a microwave cavity comprising a mechanical element. Circuits provide an opportunity to engineer nonlinear cavities, by using Josephson junctions, thereby generating quantum states of light for optomechanics experiments.
Here, we will theoretically describe an optomechanical setup where the cavity is realized by an LC circuit driven by a dc-biased Josephson junction. By engineering the nonlinearity, such a cavity becomes an effective N-level system, with $N = 2, 3, ...$, where the access to Fock states $N$ and above is blocked. Consequently, the cavity emission spectrum shows Mollow-type side peaks, analogous to an optical cavity interacting with an atom. We show that at these Mollow side peaks, the system exhibits a new, nonlinear type of optomechanical cooling. We calculate the cooling rate using the spectral density of noise due to the radiation pressure [1] and highlight how its unusual features compared to conventional optomechanics, can be explained in a dressed state picture.

[1] F. Marquardt *et.al.*, Phys. Rev. Lett. **99** (2007) 093902

HL 23.2 Tue 12:00 H 3007

**Logarithmic susceptibility of a quantum parametrically modulated oscillator** — •Daniel Boness[1], Wolfgang Belzig[1], and Mark Dykman[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

A weakly damped nonlinear oscillator modulated close to twice its eigenfrequency has two stable states, which have the same vibration amplitudes but opposite phases. The states are equally populated due to classical or quantum fluctuations.

An extra force at half the modulation frequency lifts the symmetry of the states. Even a weak force can result in a significant change of the populations, as it beats against the intensity of quantum and classical fluctuations. We develop an approach that allows us to find this population change.

We also study the effect of the extra force with frequency slightly detuned away from half the modulation frequency. For a detuning that is small compared to the switching rate the force leads to the imbalance of populations that is modulated at the frequency of the detuning. For larger detuning, the adiabatic picture breaks down and

the wells are again equally populated. However, the rates of switching between the wells is exponentially increased. We calculate the change of the logarithm of the switching rate, termed logarithmic susceptibility, using the real-time instanton method. The results are relevant for controlling parametric oscillators and their application in quantum information systems.

HL 23.3 Tue 12:15 H 3007

**Cavity optomechanics with carbon nanotube quantum dots** — •Akong N. Loh, Furkan Özyigit, Fabian Stadler, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Carbon nanotubes (CNTs) are the smallest and lightest nanomechanical beam resonators. When suspended transversally between two electrodes (Ti/Au for example) and then gated, they can act as mechanical beam resonators with large quality factors and also as quantum dots. The motion of a CNT is coupled to other degrees of freedom, such as photons, spins, and electrons. The optomechanical coupling of a single wall carbon nanotube nanomechanical resonator to a microwave cavity has been realized and quantified through optomechanically induced transparency measurements [1]. The quantum dot properties of the CNT were exploited (specifically the nonlinearity of the coulomb blockade) to significantly enhance the coupling strength [1,2]. Current work is directed towards achieving even stronger coupling and possibly groundstate cooling of the nanomechanical resonator through anti-Stokes processes. This requires significant improvement of the microwave cavity, CNT growth and transfer. All measurements are done at ∼10 mK in a dilution refrigerator.

[1] S. Blien *et al.*, Nat. Comm. **11** (2020) 1636
[2] N. Hüttner et al., Phys. Rev. Applied, in press (2023), arXiv:2304.02748

HL 23.4 Tue 12:30 H 3007

**Signatures of Josephson force in a vibrating carbon nanotube junction** — •Andreas K. Hüttel[1,2], Jukka-Pekka Kaikkonen[2], Keijo Korhonen[2], and Pertti Hakonen[2] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Low Temperature Laboratory, Dept. of Applied Physics, Aalto University, Espoo, Finland

A carbon nanotube suspended between superconducting electrodes acts simultaneously as nanomechanical resonator and as a Josephson junction. Its energy-dependent density of states and with that displacement-dependent critical current further adds to the complexity of the system, as does both mechanical and electronic nonlinearity. Measurements on such a system display complex behaviour of the vibrational resonance with respect to junction biasing. Strikingly, the resonance frequency appears to decrease in a distinct parameter region where the biasing is similar in size to the junction switching current.

Using highly parallelized Julia code, we numerically solve the coupled differential equation system of the driven (via an ac gate voltage and ac current or voltage bias) system for realistic device parameters and characterize the evolving steady state. Specific attention is given to the impact of the Josephson junction behaviour on the mechanical resonance frequency and the vibration amplitude, and on the ac signal simultaneously acting on gate and bias.

HL 23.5 Tue 12:45 H 3007

**Optimization of Flux-Tunable Microwave Resonators for Strong Single-Photon Optomechanics in Nano-Electromechanical Systems** — •Korbinian Rubenbauer[1,2], Thomas Luschmann[1,2], Kedar Honasoge[1,2], Achim Marx[1,2], Kirill G. Fedorov[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, Munich, Germany

Quantum sensing leverages quantum properties to enhance the precision of sensing applications. One promising implementation for the detection of forces or accelerations are optomechanical systems which encode the displacement of a low-frequency mechanical element onto the properties of a high-frequency optical or electromagnetic resonator. We present a flux-tunable superconducting quantum circuit with an integrated superconducting quantum interference device (SQUID), where the mechanical element is embedded in the SQUID structure. This implements a magnetic field and flux tunable optomechanical interaction with the prospect of reaching the strong single-photon coupling regime. We discuss the design concept of the device and detail its optimization. We corroborate the conceptual improvements with experimental data demonstrating the performance improvements of the microwave resonator, the optomechanical coupling and the mechanical element.

## HL 24: Graphene and 2D Materials (joint session TT/HL)

Time: Wednesday 9:30–11:15 Location: H 3007

HL 24.1 Wed 9:30 H 3007

**Static and Dynamic Properties of a 2D Superconductor Investigated by NV Center SPM** — •Sreehari Jayaram, Malik Lenger, Ruoming Peng, Rainer Stöhr, and Jörg Wrachtrup — 3rd Physics Institute, University of Stuttgart, Germany

Visualization of nanoscale dynamics in superconducting materials provides a pathway to unravel the pairing mechanisms of interacting electrons. Here, we have employed the state-of-the-art scanning NV probe technique to explore the local magnetic response of the 2D superconductor, 2H-$NbSe_2$, in which we demonstrate full dynamic sensing of vortices with high sensitivity and spatial resolution.

Utilizing this quantum probe, we present the first spatio-temporal dynamics of vortices in a 10 nm thin exfoliated 2H-$NbSe_2$, where the arrangement of the vortices show a strong correlation with the geometric confinement. Notably, we have observed the melting of vortex solids near critical temperature allowing the re-arrangement of the vortices that is governed by the cooling rate.

Additionally, our study delves into the dynamics of vortex cores, superconducting-insulator edge dynamics, and phase transitions, all unveiled through spatial-temporal noise spectroscopy with the NV probe.

HL 24.2 Wed 9:45 H 3007

**Berry Phase Effects in the Transverse Conductivity of Fermi Surfaces and its Detection With Spin Qubits and NMR** — •Mark Morgenthaler and Inti Sodemann — Universität Leipzig, Germany

The transverse conductivity of clean Fermi liquids at low frequencies displays a remarkably universal behaviour at long wavelengths: It is determined only by the geometrical radius of curvature of the Fermi surface, and does not depend on details such as the quasi-particle mass or their interactions. Here, we demonstrate that the Berry phase at the Fermi surface does not alter such long-wavelength universality by directly computing the transverse conductivity of two- and three-dimensional electronic systems with Dirac dispersions, such as those appearing in 2D graphene or in 3D Dirac semi-metals and in the bulk of 3D topological insulators. Interestingly however, such universality ceases to hold at wave-vectors comparable to the Fermi radius, and Dirac fermions display a distinct transverse conductivity from a featureless parabolic Fermion. We demonstrate that this difference originates entirely from the orbital magnetic moment of the quasi-particles induced by their Berry phases. We discuss how these effects can be probed by measuring the T1 relaxation time of spin qubits (such as NV centers) near 2D samples and for the nuclear spins measured in NMR for 3D samples.

HL 24.3 Wed 10:00 H 3007

**Fermi Velocity renormalization in graphene from large scale Quantum Monte Carlo simulations** — •Maksim Ulybyshev[1], Savvas Zafeiropoulos[2], Christopher Winterowd[3], and Fakher Assaad[1,4] — [1]Julius-Maximilians-Universität Würzburg, Germany — [2]Aix Marseille Univ, Universite de Toulon, CNRS, CPT, Marseille, France — [3]Johann Wolfgang Goethe-Universität Frankfurt am Main, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Würzburg, Germany

Through recent advancements in algorithms, we extended the capabilities of unbiased Quantum Monte Carlo (QMC) simulations up to

the lattices with spatial volume of 20808 sites. These simulations were applied to both suspended graphene and graphene on substrates, enabling direct comparison with experimental data without the need for additional extrapolations. This technique allowed us to successfully confront the numerical and experimental estimates of the Fermi velocity renormalization near the Dirac point.

Our findings validate the logarithmic divergence of the Fermi velocity, but also show the limitations of the low-energy continuum theory in quantitative description of this divergence. Additionally, our research demonstrates the significance of lattice-scale physics and higher-order perturbative corrections beyond the Random Phase Approximation (RPA) for a more accurate description of the experimental data for the Fermi velocity renormalization in suspended graphene. We also propose experimental approaches to demonstrate the role of higher-order perturbative corrections.

HL 24.4 Wed 10:15 H 3007

**Solitons induced by an in-plane magnetic field in rhombohedral multilayer graphene** — •Max Tymczyszyn, Peter Cross, and Edward McCann — Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom

The low-energy band structure of rhombohedral graphene multilayers includes a pair of flat bands near zero energy, which are localized on the surface layers of a finite thin film. Introducing an in-plane magnetic field we find that the zero-energy bands persist, and that level bifurcations occur at energies determined by the component of the in-plane wave vector that is parallel to the external field. The occurrence of level bifurcations is explained by invoking semiclassical quantization of the zero-field Fermi surface of rhombohedral graphite. We find parameter regions with a single isoenergetic contour of Berry phase zero corresponding to a conventional Landau level spectrum and regions with two isoenergetic contours, each of Berry phase $\pi$, corresponding to a Dirac-like spectrum of levels. We write down an analogous one-dimensional tight-binding model and relate the persistence of the zero-energy bands in large magnetic fields to a soliton texture supporting zero-energy states in the Su-Schrieffer-Heeger model. We show that different states contributing to the zero-energy flat bands in rhombohedral graphene multilayers in a large field are localized on different bulk layers of the system, not just the surfaces.

[1] M. Tymczyszyn, P.H. Cross, E. McCann, Phys. Rev. B 108 (2023) 115425

HL 24.5 Wed 10:30 H 3007

**Competing nematic semi-metallic and insulating states in bilayer graphene** — •Sebastian Mantilla and Inti Sodemann — Institut für Theoretische Physik, Universität Leipzig, 04107 Leipzig, Germany

The finite density of states arising from the parabolic band touching in ideal Bernal bilayer graphene leads to spontaneous symmetry-breaking instabilities driven by weak repulsive interactions. To this date, different experiments have reported conflicting states, with some reporting a gapped state and others a metallic state that spontaneously breaks lattice rotations. Using a combination of bosonization and self-consistent Hartree-Fock theory, we propose a resolution to these conflicting reports by demonstrating the existence of two closely competing states: a semi-metallic nematic state in which the parabolic band touchings spontaneously split into a pair of linearly dispersing Dirac fermions and a fully gapped state. We find that the gapped state has slightly lower energy, but the energy difference between them is highly sensitive to the interaction strength in a BCS-like fashion. Therefore, in samples with more screening, these states are even closer in energy, and their energetic balance can be tilted by other corrections, such as the trigonal warping, which tends to favour the nematic metallic states.

HL 24.6 Wed 10:45 H 3007

**Atomistic approach to correlations in multilayer graphene** — •Ammon Fischer[1], Lennart Klebl[2], Tim Wehling[2], and Dante M. Kennes[1,3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University — [2]I. Institute for Theoretical Physics, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany

Multilayer graphene has recently attracted considerable attention due to the discovery of cascades of correlated states and superconductivity driven by displacement field tunable van-Hove singularities at low densities. While experimental efforts aim to stabilize correlated phases by proximity-induced spin-orbit coupling or by increasing the number of graphene layers in the stack, first-principle guided theoretical investigations are thwarted by the strong momentum-localization of the low-energy degrees of freedom around the valleys K,K'. Here, we discuss how correlated phenomena in few-layer graphene can be resolved by atomistic weak-coupling methods including the random-phase approximation and the functional renormalization group using ab-initio derived interaction profiles. We demonstrate that the gap between phenomenological continuum model studies and atomistic investigations can be bridged by a novel Wannierization procedure that permits to relax the strong momentum-localization of the low-energy Bloch states. This enables a well-defined downloading procedure of long-ranged Coulomb interactions to the valley-local flat bands of multilayer graphene systems subject to external displacement fields.

HL 24.7 Wed 11:00 H 3007

**Pseudomagnetotransport in strained and scaled graphene** — Jia-Tong Shi, Aitor Garcia-Ruiz, and •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Graphene is highly susceptible to externally applied mechanical deformation due to its atomic thinness. As such, strained graphene has long been studied both theoretically and experimentally. Among all interesting predictions, the pseudo-magnetic field in graphene under properly designed strain fields, giving rise to effects equivalent to graphene under a strong external magnetic field on the order of 10 Tesla [1], is perhaps one of the most intensively discussed topics. Despite the experimentally observed pseudo-Landau levels due to strong pseudo-magnetic fields in graphene bubbles [2] and ripples [3], transport experiments showing strong pseudo-magnetic fields in strained graphene have so far been missing. To provide reliable guides to possible future pseudo-magnetotransport experiments on strained graphene, here we perform quantum transport simulations considering triaxially strained graphene using the scalable tight-binding model [4]. Numerical examples of transverse pseudo-magnetic focusing and pseudo-quantum Hall effect will be shown.

[1] F. Guinea, M. I. Katsnelson, A. K. Geim, Nat. Phys. **6** (2010) 30
[2] N. Levy *et al.*, Science **329** (2010) 544
[3] S. Y. Li *et al.*, Phys. Rev. Lett. **124** (2020) 106802
[4] M.-H. Liu, *et al.*, Phys. Rev. Lett. **114** (2015) 036601

# HL 25: Oxide Semiconductors I

Time: Wednesday 9:30–12:45 Location: ER 325

HL 25.1 Wed 9:30 ER 325

**Photoluminescence study of corundum-like $\alpha$-$Ga_2O_3$** — •Lennart Hölzer[1], Elias Kluth[1], Rüdiger Goldhahn[1], Dae-Woo Jeon[2], Kazuaki Akaiwa[3], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Korean Institute of Ceramic Engineering and Technology, Jinju, South Korea — [3]Department of Information and Electronics Engineering, Tottori University, Japan

$Ga_2O_3$ is a polymorphic ultra-wide band gap semiconductor with promising usage in power electronic devices like MOSFETs and Schottky diodes. Due to its thermodynamical stability, research has primarily focused on the stable $\beta$-phase.

Despite being metastable, $\alpha$-$Ga_2O_3$ is just as interesting with an even wider band gap of $\approx 5.6$ eV. Band gap engineering also has been proven possible in a range of about 3.7 to 9 eV by alloying with Al, In or Ti. This enables applications in devices such as solarblind photodetectors and FETs.

There is, nevertheless, a significant lack of knowledge of the optical properties. To investigate these, $c$-plane and $m$-plane $\alpha$-$Ga_2O_3$ samples grown on sapphire substrates by HVPE and mist-CVD were studied using low temperature photoluminescence. A luminescence band in the UV-region at 3.75 eV was identified. The correlation of temperature and luminescence intensity was evaluated, yielding activation energies in the magnitude of the donor binding energy.

HL 25.2 Wed 9:45 ER 325

**Red shift of the absorption onset in orthorhombic $\kappa$-$(In_xGa_{1-x})_2O_3$ alloys** — •Elias Kluth[1], Alexander Karg[2], Martin Eickhoff[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Institut für Festkörperphysik, Universität Bremen, Germany

The polymorphic ultra-wide band gap semiconductor $Ga_2O_3$ is of high research interest as it offers potential in power electronics like MOSFETs, MeSFETs or Schottky diodes as well as in solar-blind UV detectors, and many more.

While previous research has mostly focused on the stable $\beta$- or the metastable $\alpha$-phase, the orthorhombic $\kappa$-$Ga_2O_3$ is only poorly explored. This phase is predicted to be polar with a high spontaneous polarisation, potentially even higher than GaN, making it interesting for applications such as high electron-mobility transistors (HEMTs). Alloying $\kappa$-$Ga_2O_3$ with indium further extends these possibilities. For a successful device implementation, an understanding of the optical properties is essential.

Here, spectroscopic ellipsometry in the visible-ultraviolet range is perfomed on $\kappa$-$(In_xGa_{1-x})_2O_3$ with $x \leq 0.16$, grown by MBE (molecular beam epitaxy) on $c$-plane sapphire substrates, to obtain the complex dielectric function. An evaluation of the dielectric function yields a strong red shift in the absorption onset with increasing indium content ($x$).

HL 25.3 Wed 10:00 ER 325

**Comparative study of temperature-dependent bandgap transitions in $Ga_2O_3$ polymorphs** — •Benjamin M. Janzen[1], Nima Hajizadeh[1], Moritz Meissner[1], Marcella N. Marggraf[1], Conrad V. Hartung[1], Alwin Wüthrich[1], Nils Bernhardt[1], Felix Nippert[1], and Markus R. Wagner[2] — [1]Technische Universität Berlin — [2]Paul-Drude-Institut für Festkörperelektronik

The temperature dependence of the optical bandgap has rarely been investigated experimentally for the different polymorphs of $Ga_2O_3$. A direct comparison of the temperature dependence as well as the electron-phonon coupling strengths is made considerably more difficult by the different experimental methods (e.g., reflection spectroscopy, absorption spectroscopy or ellipsometry) used to study the various polymorphs. In particular, there is no study in the literature that provides a self-consistent comparison between the band gap values, the averaged phonon energies and the electron-phonon coupling strengths of the different polymorphs using the same experimental technique. We provide an experimental study to investigate the electronic bandgap transitions in monoclinic $\beta-$, orthorhombic $\kappa-$, rhombohedral $\alpha-$, defective-spinel $\gamma$- and cubic bixbyite $\delta-Ga_2O_3$ as a function of the sample temperature. Temperature-dependent UV photoluminescence excitation (PLE) spectroscopy is employed in the temperature range between 5 K and 300 K and the temperature dependencies are discussed regarding the energy bandgap, the effects of electron-phonon coupling and the averaged phonon energies.

HL 25.4 Wed 10:15 ER 325

**Optical phonon modes in $LaInO_3$: Lattice dynamics and complete polarization analysis of Raman-active modes** — •Hans Tornatzy[1], Roland Gillen[2], Zbigniew Galazka[3], Oliver Brandt[1], Manfred Ramsteiner[1], and Markus R. Wagner[1] — [1]Paul-Drude-Institut, Berlin — [2]Friedrich-Alexander Universität Erlangen-Nürnberg — [3]Leibniz-Institut für Kristallzüchtung, Berlin

$LaInO_3$ is part of the family of $ABO_3$ perovskites, and is considered promising for next generation devices such as for power electronics due to its band gap of about 4.5 eV. A detailed knowledge of phonon modes in $LaInO_3$ is important as they determine a number of material properties such as the mechanical and elastic properties, thermal transport and carrier dynamics, phonon-assisted optical excitations, and many more. However, little is known about the vibrational properties of this material. In this study, we investigate the lattice dynamics by polarization- and angle-resolved Raman spectroscopy and density functional theory (DFT). We experimentally observe all but one of the Raman active modes and compare them to our simulated values from DFT. Furthermore, we derive the phonon dispersion relation along the high symmetry directions in reciprocal space and depict the oscillation patterns for selected phonons at the $\Gamma$ point. Finally, we determine the relative Raman tensor elements of the observed modes from the angular dependence of their corresponding scattering efficiencies.

HL 25.5 Wed 10:30 ER 325

**Raman active phonon modes of single-domain orthorhombic $\kappa$-$Ga_2O_3$** — •Alwin Wüthrich[1], Benjamin M. Janzen[1], Hiroyuki Nishinaka[2], Roland Gillen[3], and Markus R. Wagner[1,4] — [1]Technische Universität Berlin — [2]Kyoto Institute of Technology — [3]Friedrich-Alexander Universität Erlangen-Nürnberg — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin

Next-generation electronic and photonic devices require advanced materials with tailored properties. The orthorhombic $\kappa$-phase of $Ga_2O_3$ features an ultrawide bandgap around 5 eV, a large spontaneous polarization along the c-axis and ferroelectric behaviour. A major obstacle for device applications based on $\kappa$-$Ga_2O_3$ is the formation of rotational domains. Established growth techniques like MBE, MOVPE, PLD and mist CVD have so far only produced rotational-domain samples, where orthorhombic domains with sizes up to 200 nm align along three preferential directions that are 120°-rotated with respect to each other. Most recently, the growth of single-domain $\kappa$-$Ga_2O_3$ on orthorhombic $\varepsilon$-$GaFeO_3$ was demonstrated by mist CVD, resulting in a lattice mismatch as low as 1%. We present comprehensive Raman spectra of single-domain $\kappa$-$Ga_2O_3$, using a set of dedicated polarization geometries to resolve more than 100 of the 117 optical Raman-active modes experimentally. Moreover, we present the angular dependent Raman scattering intensities for excitation of the c-plane, proving the single-domain orthorhombic nature of the investigated thin film.

HL 25.6 Wed 10:45 ER 325

**Determination of self-trapped exciton emission bands in $Ga_2O_3$ polymorphs** — •Nima Hajizadeh[1], Benjamin M. Janzen[1], Moritz Meissner[1], Marcella N. Marggraf[1], Conrad V. Hartung[1], Alwin Wüthrich[1], Nils Bernhardt[1], Felix Nippert[1], and Markus R. Wagner[2,1] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V.

Several temperature and excitation dependent photoluminescence (PL) and excitation (PLE) spectra are published for the thermodynamically stable $\beta$ phase. In addition, a large number of theoretical calculations allow the assignment of observed emission bands. Accordingly, the UV bands in $\beta$-$Ga_2O_3$ are associated with the recombination of a self trapped hole (STH) and bound electrons. Such clear experimental assignments of optical bands for the different $Ga_2O_3$ polymorphs do not yet exist. Using temperature-dependent PL and PLE spectroscopy, we provide a study to investigate emission bands of monoclinic $\beta$-, orthorhombic $\kappa$-, rhombohedral $\alpha$-, defective-spinel $\gamma$- and cubic bixbyite

$\delta$-$Ga_2O_3$ as a function of excitation and temperature. Based on these spectra, a possible experimental identification of STH emission bands for different $Ga_2O_3$ polymorphs will be discussed. Furthermore, this evaluation may be supported by a correlation between the experimental stokeshifts and the theoretically calculated self-trapping energies in the literature, which would allow the detection and energetic determination of these excitons.

**30 min. break**

HL 25.7 Wed 11:30 ER 325

**Nonlinear bond length change 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, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

CuI is one of the most promising transparent p-type semiconductors with various applications from diodes to solar cells, including also flexible electronics [1]. Among numerous doping and alloying attempts, anion substitution with bromide can be used to tailor the free hole concentration in functional layers enabling optimized performance of active devices such as pn-diodes or transistors [2]. Using X-ray absorption spectroscopy, the element-specific 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 near edge region is used to identify the presence and amount of oxygen contamination of the samples. 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 observed for III-V and II-VI zincblende alloys [3].

[1] Grundmann et al., *Phys. Status Solidi A* **210**, No. 9, 1671 (2013)
[2] Yamada et al., *Adv. Funct. Mater.* **30**, 2003096 (2020)
[3] Schnohr, *Appl. Phys. Rev.* **2**, 031304 (2015)

HL 25.8 Wed 11:45 ER 325

**Magnetostriction in spinel zinc ferrite revisited: A first-principles investigation** — •Daniel Fritsch — Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

Magnetostriction describes the property of materials to change its length or volume when going from randomly oriented magnetic moments to an ordered state by placing it in a magnetic field. Typically, these changes are of the order $10^{-6}$ or less, however, some materials have been shown to show larger magnetostriction, and have consequently been employed for sensor applications.

Among the material class of spinel ferrites, $CoFe_2O_4$ shows very large magnetostriction [1], and a recent experimental investigation reported similar in $ZnFe_2O_4$. Here, we revisit magnetostriction in $ZnFe_2O_4$ by means of first-principles calculations, employing density functional theory and hybrid exchange and correlation functionals [2], together with a recently devised method to speed-up these calculations [3]. The obtained results will be discussed with respect to available experimental findings and complement our knowledge about magnetostriction in spinel ferrites.

[1] D. Fritsch and C. Ederer, Phys Rev B **82**, 104117 (2010), Phys. Rev. B **86**, 014406 (2012).
[2] D. Fritsch, J. Phys.: Condens. Matter **30**, 095502 (2018).
[3] D. Fritsch, Appl. Sci. **12**, 2576 (2022).

HL 25.9 Wed 12:00 ER 325

**Screening of contact metals for optimized performance of $\alpha$-$Ga_2O_3$ based Schottky Barrier Diodes** — •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 $\alpha$-$Ga_2O_3$:Sn based Schottky barrier diodes with exceptional current rectification ratios of up to 8 orders of magnitude and high mean barrier heights of up to 2.53 eV. By evaluating various Schottky metals, we find that reactively sputtered $Pt/PtO_x$ yields the best performing Schottky barrier diodes [1]. We further show temperature dependent IV-measurements in the range of 40 K-400 K that are in agreement with the thermionic emission model. The effective barrier heights could accurately be fitted using the laterally inhomogeneous barrier model [2].
In recent years the metastable corundum-structured $\alpha$-phase of $Ga_2O_3$ has shown to have promising physical properties. With a bandgap of 5.3-5.6 eV [3,4] and a predicted breakdown field of 10 MV/cm it surpasses the theoretical limits of $\beta$-$Ga_2O_3$ in terms of Baliga's figure of merit [4]. Further, $\alpha$-$Ga_2O_3$ is isostructural to $\alpha$-$Al_2O_3$ and hence epitaxial growth on cost-efficient sapphire substrates is feasible.

[1] S. Koepp *et al.*, J. Vac. Sci. Technol. A 41, 043411 (2023)
[2] D. Splith *et al.*, Phys. Status Solidi A, 218: 2100121 (2021)
[3] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[4] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)

HL 25.10 Wed 12:15 ER 325

**Tailoring analog $TiN/SiO_x/Cu/SiO_x/TiN$ memristive devices through experiments and simulations** — •Rouven Lamprecht[1], Tobias Gergs[2], Luca Vialetto[2], Finn Zahari[1], Richard Marquardt[1], Jan Trieschmann[2], and Hermann Kohlstedt[1] — [1]Chair of Nanoelectronics, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Germany — [2]Chair of Theoretical Electrical Engineering, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Germany

Memristive devices for neuromorphic circuits are an emerging nanotechnology promising for bioinspired computing architectures. Due to their voltage-dependent change in resistance, memristive devices can be considered as electronic pendants to synapses in the nervous system. In this study, we combine an experimental and modeling approach to systematically characterize the electrical properties of memristive devices, which were fabricated using different process methods with varying parameters. Experimental data provides local measurements of current-voltage (I-V) characteristics demonstrating analog switching of the $TiN/SiO_x/Cu/SiO_x/TiN$ memristive devices. Monte Carlo simulations provide insights into the fabrication conditions by modeling the deposition source (thermal evaporation and magnetron sputtering) as well as the deposited thin film composition. As a result of the study, we correlate the measured electrical device properties with simulated deposition properties to provide insights into the key operational conditions influencing the memristive behavior.

HL 25.11 Wed 12:30 ER 325

**Two-dimensional electron gas in polar-discontinuity doped $LaInO_3/BaSnO_3$ heterostructure grown by plasma-assisted molecular beam epitaxy** — •Georg Hoffmann[1], Martina Zupancic[2], Martin Albrecht[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Transparent semiconducting oxides (TSO's) are key players for new (opto-)electronic devices. In the search for suitable TSOs, the wide-bandgap semiconductor $BaSnO_3$ has been reported to provide the highest room temperature electron mobilities within the perovskite oxides - up to 320 $cm^2/Vs$ for La doped bulk material [1]. Interfacing the undoped, nonpolar $BaSnO_3$ with the closely lattice-matched, polar $LaInO_3$ is predicted to create a two-dimensional electron gas (2DEG) with a charge carrier density of up to $2\times10^{14}/cm^2$ due to polar-discontinuity doping [2]. Here, we demonstrate the adsorption-controlled growth of $LaInO_3/BaSnO_3$ heterostructures grown by plasma-assisted molecular beam epitaxy. The formation of the 2DEG at the $LaInO_3/BaSnO_3$ interface is confirmed by capacitance-voltage and van der Pauw-Hall measurements. The extracted sheet electron concentrations above $2\times10^{13}/cm^2$ and RT electron mobilities above 100 $cm^2/Vs$ pave the way for further device studies.

[1] H. J. Kim et al., Appl. Phys. Express, 5, 061102 (2012). [2] K. Krishnaswamy et al., Appl. Phys. Lett. 108, 083501 (2016).

# HL 26: 2D Materials and Heterostructures: Quantum Emitters and Defects

Time: Wednesday 9:30–12:15 Location: EW 201

HL 26.1 Wed 9:30 EW 201

**Spin Dynamics of Quantum Sensors Based on Hexagonal Boron Nitride** — •Paul Konrad[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

Colour centres in solid-state materials show great potential in quantum information technology and sensing applications. The lately discovered negatively charged boron vacancy ($V_B^-$) in hexagonal boron nitride (hBN)[1] has shown that the defect exhibits a spin-triplet ground state with spin-dependent photoluminescence. The system can be exploited in terms of its application as temperature, magnetic field, and pressure sensor [2,3] which extends the already known applications of e.g. NV-centers in diamond not only due to its 2D character but also by highly improved temperature sensing especially at low temperatures.

Here we present new insights into the spin dynamics of $V_B^-$ in form of measurements of ground-state repopulation after pulsed laser excitation. For these studies we record transient photoluminescence with sub-nanosecond accuracy and determine the influence of the relaxation dynamics on the coherent control of the quantum system. This information can be used to optimize pulse timing.

[1] Gottscholl et al., *Nat. Mat.*, **19**, 5, 540 (2020).
[2] Gottscholl et al., *Sci. Adv.*, **7** (14), eabf3630 (2021).
[3] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).

HL 26.2 Wed 9:45 EW 201

**Dephasing Dynamics in Defect Centers of Hexagonal Boron Nitride Probed by Time-Resolved Cathodoluminescence Spectroscopy** — •Nahid Talebi[1,2], Masoud Taleb[1,2], Paul Bittorf[1], Maximilian Black[1], Mario Hentschel[3], and Kourosh Esmaeeli Koshkoie[3] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Birkenweg 20 — [3]34th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Defect centers in hexagonal boron nitride (hBN) have been extensively explored as room-temperature single-photon sources. The electronic structures of these defects exhibit strong coupling to phonons, as evidenced by the observation of phonon sidebands in both photoluminescence and cathodoluminescence spectra, and as reported in the literature. However, the dynamics of the electron-phonon coupling as well as phonon-mediated dephasing of the color centers in hBN have remained unexplored. Here, we apply a novel time-resolved CL spectroscopy technique (Nature Physics 19, 869*876 (2023)) to explore the population decay to phonon states and the dephasing time T2 with sub-femtosecond time resolution. We demonstrate an ultrafast dephasing time of only 200 fs and a population decay of approximately 700 fs at room temperature, in contrast with all-optical time-resolved photoluminescence techniques that report a decay of a few nanoseconds. This behavior is attributed to an efficient excitation of coherent phonons polaritons in hBN with electron beams that results in faster dephasing of electronic transitions.

HL 26.3 Wed 10:00 EW 201

**Radial quasi Bound States in the Continuum fabricated from Hexagonal Boron Nitride** — •Connor Heimig, Jonas Biechteler, Thomas Weber, Luca Sortino, and Andreas Tittl — Chair in Hybrid Nanosystems, Nanoinstitute Munich, Faculty of Physics, Ludwig-Maximilians-Universität München, 80539 Munich, Germany

We present a novel class of optical metasurfaces through the integration of the radial quasi Bound State in the Continuum (qBIC) concept into the realm of 2D van der Waals materials. Our design is underpinned by Radial qBICs, arising from structural asymmetry in a ring of trapezoid pair resonators fabricated from hexagonal Boron Nitride (hBN).

Overcoming the trade-off between refractive index and optical losses, symmetry-broken qBICs efficiently suppress radiation losses from hBN, enabling high-Q resonances across the entire visible spectrum. Leveraging the unique properties of a low-refractive index van der Walls material such as hBN, allows the development of a novel nanophotonic platform for enhanced light-matter interaction. This integrated approach further establishes an experimental foundation for the implementation of hBN as a photonic medium for metaoptics, offering prospects for compact, spectrally selective, and polarization-invariant metadevices for diverse on-chip photonics applications.

HL 26.4 Wed 10:15 EW 201

**Controlling the emission intensity of hBN emitters by graphene gates** — •Corinne Steiner[1,2], Rebecca Rahmel[1], Frank Volmer[3], Patricia Pesch[1], Kenji Watanabe[4], Takashi Taniguchi[5], Bernd Beschoten[1], Christoph Stampfer[1,2], and Annika Kurzmann[1,6] — [1]JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Germany — [2]Peter Grünberg Institute, FZ Jülich, Germany — [3]AMO GmbH, Aachen, Germany — [4]Research Center for Functional Materials, NIMS, Japan — [5]International Center for Materials Nanoarchitectonics, NIMS, Japan — [6]Physics Institute 2, University of Cologne, Germany

Two-dimensional hexagonal boron nitride is a host material for bright and stable single-photon emitters. By applying strain or electric fields, their emission properties can be tuned, rendering them promising candidates for quantum photonic applications [1,2]. Here, we present voltage-dependent photoluminescence measurements of a quantum emitter in dual-graphene-gated hBN, showing a gate-controllable, steplike, fivefold increase in emission intensity. Furthermore, we observe a correlation between the reported increase of emitter intensity and the direction of the leakage current through the hBN. This suggests photo-induced tunneling processes within the hBN as an explanation for the observed intensity switching. Thus, our results are a step towards understanding the charge dynamics between graphene gates and hBN quantum emitters.

[1] Nano Lett. 18, 4710 (2018)
[2] Light: Science & Applications 11, 186 (2022)

HL 26.5 Wed 10:30 EW 201

**Excited state geometry relaxation of point defects in monolayer hexagonal boron nitride** — •Alexander Kirchhoff, Thorsten Deilmann, and Michael Rohlfing — University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Straße 10, 48149 Münster

Point defects in hexagonal boron nitride (hBN) are often discussed as single-photon emitters for quantum technologies. Understanding the dependence of electronic and optical properties on the geometry might help to identify the atomic structure of the defects and is also crucial in order to make these emitters applicable. Here, we study three defects in a monolayer of hBN, namely $C_BV_N$, $C_BC_N$ and $C_BO_N$, from an ab initio approach. We use (constrained) density functional theory to obtain optimal geometries of the electronic ground state and the first excited state, and then refine quasi-particle energies and optical excitation energies using a *GW* and BSE based appraoch. All three defect systems host transitions between deep lying defect states. We find the lowest defect exciton of $C_BC_N$ at $\sim 4\,\mathrm{eV}$ and for the other two defects at $\sim 2\,\mathrm{eV}$ with significant Stokes shifts of $0.2\,\mathrm{eV}$ and $0.7\,\mathrm{eV}$, respectively.

HL 26.6 Wed 10:45 EW 201

**Understanding the Role of Defects in WS2 layer in contact with ZnO substrate** — •Dedi Sutarma and Peter Kratzer — Department of Physics, University of Duisburg-Essen

The remarkable properties of two-dimensional (2D) materials have garnered significant attention in recent years, and understanding their fundamental behavior is critical for developing next-generation technologies. In this study, we investigate the microscopic behavior of a 2D material, $WS_2$, with ZnO (1 -1 0 0) taking the role as the substrate as well as charge injection layer in this van der Waals (vdW) heterostructures. Using density functional theory calculations, we examine the structural and optoelectronic properties of the $WS_2$/ZnO, including the impact of point defects. Herein, band alignment of the heterojunction is found to be type I, with the larger band gap in ZnO, which is desirable for using ZnO as an electron injector for radiative recombination in monolayer $WS_2$ forming the active layer in a light-emitting device. Our results demonstrate that defects can significantly modulate the electronic properties of the interface, including band alignment and charge transfer. Furthermore, absorption and Raman spectra are

calculated to understand the optical behavior of this system. This work is funded by DFG IRTG 2803 and NSERC CREATE.

**15 min. break**

HL 26.7 Wed 11:15 EW 201

**Enhanced light-matter interaction in self-assembled photonic-defect nanocavities with a TMDC monolayer as active material** — •Aris Koulas-Simos[1], Chirag Palekar[1], Kartik Gaur[1], Imad Limame[1], Ching-Wen Shih[1], Bárbara Rosa[1], Cun-Zheng Ning[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Department of Electronic Enginnering, Tsinghua University, Beijing 100084, China

Micro- and nanolasers utilizing TMDCs as active materials have been gaining significant research popularity for novel photonic applications. Here, we report on the fabrication of multiple self-assembled photonic-defect nanocavities in a single, fully encapsulated $WSe_2$ monolayer embedded in a dielectric distributed Bragg reflector (DBR) structure. The bubble-like Gaussian defect nanocavities provide tight optical lateral confinement and produce diameter-dependent optical signatures distinguishing them from the planar DBR-section, as validated in $\mu$PL-measurements and numerical cavity simulations. Last but not least, optical power-dependent studies at cryogenic temperatures reveal an enhanced light matter-interaction through a pronounced kink in the I/O-curve and a slight linewidth narrowing for two specific devices.

HL 26.8 Wed 11:30 EW 201

**Optoelectronic energy conversion based on atom scale and sustainable device architectures** — •Maximilian A. Gruber, Alexander Hötger, and Alexander W. Holleitner — Walter-Schottky-Institute, TU Munich

Two-dimensional (2D) materials and heterostructures allow the exploration of fundamental quantum phenomena and advancing optoelectronics. Our work showcases a methodology for the integration of atomistic defects into 2D heterostructures, aiming to address the open-circuit voltage of single to few defects in a vertical tunneling device, revealing the potential of single-vacancy tunneling devices as atomic-scale photodiodes [1]. Moreover, we investigate the dynamics of hot charge carriers in atomically thin heterostructures via photocurrent and photovoltage experiments aiming to unravel the mechanisms of generation, transport and relaxation of hot carriers.

[1] A. Hötger *et al.* Photovoltage and photocurrent absorption spectra of sulfur vacancies locally patterned in monolayer $MoS_2$. Nano Letters accepted (2023)

HL 26.9 Wed 11:45 EW 201

**Substrate-dependent quantum and magneto-optical properties of $WSe_2$ single-photon emitters** — •Bárbara Rosa[1], Caique Serati de Brito[2], Cesar Ricardo Rabahi[2], Ingrid D. Barcelos[3], Yara Galvão Gobato[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Department of Physics, Federal University of São Carlos, São Carlos, Brazil — [3]Brazilian Synchrotron Light Laboratory, Brazilian Center for Research in Energy and Materials, Campinas, Brazil

Two-dimensional (2D) van der Waals materials have arisen as a novel platform to explore the characteristics of non-classical light throughout the fabrication of single-photon emitters (SPEs). Their large range of emission wavelengths, site-controllability, and the accessible properties tuning by engineered strain and defects, turning them into potential candidates for several applications. Here, we investigate the quantum-optical properties of $WSe_2$ SPEs generated on different substrates. Interestingly, by conducting off- and quasi-resonant optical excitation, we observe a substrate dependence on the number of quantum emitters and their extracted linewidths, in which the doped surfaces command the properties of defect-states created in $WSe_2$ SPEs. Similar effects are also observed in the multi-photon suppression determined through photon correlation measurements. In addition, we performed magneto-photoluminescence studies, where extracted g-factors for the systems above show a remarkably substrate-dependent response.

HL 26.10 Wed 12:00 EW 201

**Monolayer-based single photon source in an open cavity featuring 65 % brightness and quantum coherence** — •Jens-Christian Drawer[1], Victor Nicolaevich Mitryakhin[1], Hangyong Shan[1], Sven Stephan[1,2], Falk Eilenberger[3], Martin Silies[2], Carlos Anton-Solanas[1], Martin Esmann[1], and Christian Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]Hochschule Emden/Leer, Emden, Germany — [3]Friedrich-Schiller-Universität Jena, Jena, Germany

In the fields of quantum communication and computation, non-classical light in the form of single photons is of critical importance. A promising candidate for single-photon sources are atomically thin crystals of layered van der Waals materials, although their performance has thus far been inferior to other state-of-the-art sources built from bulk crystals and semiconductors, such as InAs quantum dots. Here we present results from a single-photon source based on an atomically thin layer of $WSe_2$ coupled to an open-cavity optical resonator and operated at a temperature of 3.2 K. A finely tuned cavity enables selective Purcell-enhanced emission with efficient quasi-resonant emitter excitation. We characterize its single-photon purity to be $g^{(2)}(0) = 0.047 \pm 0.007$, measured by the second-order coherence function $g^{(2)}$ in the Hanbury Brown and Twiss setup under pulsed operation, and observe a first-lens brightness of $65 \pm 4$ % of linearly polarized photons. A first observation for this material, to our knowledge, was made in the form of quantum interference between successively emitted photons in a Hong-Ou-Mandel experiment.

## HL 27: Quantum Dots and Wires: Optics II

Time: Wednesday 9:30–11:30 Location: EW 202

HL 27.1 Wed 9:30 EW 202

**Single mode coupled emission of resonant and cw excited GaAs quantum dots** — •Martin Kernbach[1], Sophia Fuchs[2], Julian Siller[2], and Andreas W. Schell[1] — [1]Johannes Kepler University Linz — [2]Leibniz University Hannover

Advanced quantum technologies like computing or sensing demand for deterministic bright sources of single indistinguishable photons. In order to provide quantum light of isolated systems properly usable for quantum applications, an efficient excitation and extensive collection in a single mode is required. Single molecules and cavity confined quantum dots are convenient sources. The coupling to the excited state is maximized on resonance, but challenges the usability of the emitter due to the effort for separation of the optical excitation mode from the mode of emission. A temporal, spacial, spectral, or combined method for separation is typically used.

Here we present a realization of a single emitter under resonant excitation in a confocal setup with a polarization filtered emission coupled into a single mode fiber. The optical path is free beam along a one meter long stick which dives the objective lens and scanning stage into a liquid helium reservoir. For resonant cw excitation of GaAs semiconductor quantum dots a SNR of polarization suppression up to 400 and count rates of 2 Mcps are archived by using a collecting lens with NA 0.68 only. Under this scheme further investigations regarding the blinking behavior are possible as well as probing alternative emitters like single molecules.

HL 27.2 Wed 9:45 EW 202

**Diameter dependence of light absorption enhancement in GaAs nanowires evidenced by photoluminescence spectroscopy** — •Francisca Marín, Ijaas Mohamed, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Semiconductor nanowires have attracted increasing interest for photovoltaic applications, among other reasons because the absorption of light can be enhanced compared to planar layers by the appropriate geometric design of nanowire arrays. This benefit is due to the more complex coupling of light with nanowires whose dimensions are

of similar scale as the light wavelength. In fact, light absorption in nanowire arrays depends sensitively on the combination of wavelength and nanowire diameter, spacing, as well as length. This phenomenon has been extensively investigated by simulations, but experimentally it is challenging to probe light absorption in nanowires, in particular in single nanowires. Here, we use photoluminescence spectroscopy to study the effect of the diameter of highly phase-pure GaAs nanowires on light absorption. Our key idea is that the nature of carrier recombination depends on carrier density, which in turn is affected by the absorption of the exciting laser light. We investigated nanowires with diameters in the range 60-160 nm and find a clear absorption enhancement with a maximum for a diameter of 80 nm.

HL 27.3 Wed 10:00 EW 202

**Improving the Positioning Accuracy of Quantum Dots in Circular Bragg Grating Resonators Using Hyperspectral Imaging** — •Constantin Krause, Quirin Buchinger, Aileen Zhang, Giora Peniakov, Andreas Pfenning, Tobias Huber-Loyola, and Sven Höfling — Julius-Maximilians-Universität Würzburg, Lehrstuhl für Technische Physik, Würzburg, Deutschland

Self-assembled semiconductor quantum dots (QDs) are a well-studied source of single or entangled photons. To enhance their emission properties, QDs can be embedded in micro resonators, e.g. circular Bragg grating resonators (CBGs). To select QDs with the desired wavelength and determine their position, we use hyperspectral imaging. With this method the QDs are first mapped and subsequently the CBGs are defined via E-beam lithography.

To increase our measurement efficiency, we developed a fully automated measurement routine that allows us to measure twice the area in the same amount of time. We reduced the image distortion by modifying our setup and we investigated various designs of markers that we use to span a reference coordinate system. These improvements have increased the positioning accuracy of the QDs, enabling us to observe systematic errors in the position determination. We compensated for these errors using post-processing image correction algorithms. This further increased the positioning accuracy of the CBGs around the QDs to around 20 nm. We demonstrate the increased accuracy with measurements on InGaAs QDs embedded in a GaAs membrane.

HL 27.4 Wed 10:15 EW 202

**Investigation of Purcell Enhancement of Telecom-Wavelength Semiconductor Quantum Dots in Open Cavities** — •Nam Tran[1], Julian Maisch[1], Jonas Grammel[2], Julia Wecker[1], Thomas Herzog[1], Robert Sittig[1], Ponraj Vijayan[1], Michael Jetter[1], Simone Luca Portalupi[1], David Hunger[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]Physikalisches Institut, Karlsruher Institut für Technologie (KIT), Karlsruhe,

Single photon sources operating at telecom wavelength play a central role in quantum information, in particular when long-distance implementations are targeted. Highly promising candidates are semiconductor quantum dots (QD). Cavity quantum electrodynamics is often used to tailor the emission properties and, in case of photon sources, enhance their performances. However, limiting factors like spatial and spectral mismatch can be detrimental to the cavity-emitter interaction. Using open, tunable fiber cavities one can overcome these limitations. Here, we made a thorough investigation on how the ratio between the cavity and emitter linewidth, and unwanted mechanical vibrations can affect the achievable Purcell factor in open fiber/ semiconductor cavities embedding semiconductor QDs emitting in the telecom O- and C-band. Moreover, deterministic positioning of individual QDs enables the direct comparison of the optical properties within and outside the cavity.

**15 min. break**

HL 27.5 Wed 10:45 EW 202

**Quantum dot single-photon source in the telecom C-band with high brightness and indistinguishability** — •Wolfgang Fischer, Raphael Joos, Stephanie Bauer, Christian Rupp, Ponraj Vijayan, Michael Jetter, Simone L. Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

High efficiency sources of non-classical light in the telecom C-band represent a key building block in long-distance, fiber-based, quantum technology implementations, as quantum information and cryptography. Bright emission of pure single photons, with high coherence represent properties generally required in those quantum applications. In this work, we present a telecom C-band single-photon source consisting of an InGaAs quantum dot (QD) coupled to a circular Bragg grating (CBG). Under coherent excitation via the SUPER scheme as well as under incoherent, phonon-assisted excitation a high single photon purity as well as an excellent brightness is achieved. Simultaneously, a high indistinguishability is shown, supported by the CBG causing a Purcell enhancement. In order to further boost the indistinguishability, we implement a sub-GHz etalon filter representing the line width of the filtered source. Consequently, a further improvement of the indistinguishability as well as single photon purity is observed combined with still high brightness [1]. [1] Joos, R., arXiv:2310.20647v1, 2023

HL 27.6 Wed 11:00 EW 202

**Sending polarization-entangled photon pairs from semiconductor quantum dots through telecommunication fiber networks** — •Stefan Kazmaier[1], Tim Strobel[1], Tobias Bauer[2], Marlon Schäfer[2], Ankita Choudhary[3], Nand Lal Sharma[3], Raphael Joos[1], Cornelius Nawrath[1], Weijie Nie[3], Ghata Bhayani[3], Andre Bisquerra[1], Caspar Hopfmann[3], Simone L. Portalupi[1], Christoph Becher[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Science and Technology ($IQ^{ST}$) 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

Enabling fiber-based distribution of entangled single photons is crucial for advancing quantum repeater-based quantum communication. Semiconductor quantum dots (QDs) offer on-demand polarization-entangled photon pairs, but their near-infrared emission hinders telecommunication network compatibility. Here, compatibility is achieved by employing quantum frequency conversion (QFC). We show the conservation of polarization entanglement after QFC of the biexciton emission, making it compatible to telecommunication networks. This is utilized to prove high entanglement fidelity after propagation through a 35 km urban fiber network. Also, entanglement conservation is cofirmed after back conversion in a second QFC to 780 nm preparing an interface for a Rb-based quantum memory.

HL 27.7 Wed 11:15 EW 202

**Progress in Telecom C Band Single Photons from Semiconductor Quantum Dots** — •Daniel Vajner[1], Paweł Holewa[2,3], Emilia Zieba-Ostój[2], Maja Wasiluk[2], Martin van Helversen[1], Lucas Rickert[1], Aurimas Sakanas[4], Alexander Huck[3], Kresten Yvind[3], Niels Gregersen[3], Anna Musiał[2], Paweł Mrowinski[2], Marcin Syperek[2], Elizaveta Semenova[1,3], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technical University of Berlin, 10623 Berlin, Germany — [2]Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]Technical University of Denmark, Kongens Lyngby 2800, Denmark — [4]Quantum Foundry Copenhagen

We report progress towards high quality semiconductor quantum dot single photons at Telecom C-band wavelengths. This includes recent work demonstrating the coherent on-demand generation of indistinguishable photons from single QD devices consisting of InAs/InP QD-mesa structures heterogeneously integrated with a metallic reflector on a silicon wafer [1]. Furthermore, we show new experimental results which extend the employed two-photon-resonant excitation by using chirped excitation laser pulses as well as by adding a stimulation laser pulse resonant with the biexciton.

[1] Vajner, Daniel A., et al. arXiv preprint arXiv:2306.08668 (2023).

## HL 28: Focus Session: Heat transport at the nanoscale: theory meets experiment

Tailoring heat transport is fundamental in the design of semiconducting devices. Over the last decades, tremendous progress has been made in understanding the atomistic mechanisms that determine heat transport at the macro- and the nanoscale, as well as at interfaces. For the latter case, low-dimensional and non-epitaxial materials can lead to ultra-low, directional or topological phonon transport. Largely, these advances were enabled by the development of novel experimental nanoscale measurements and improved first-principles techniques covering the different transport regimes. The focus session brings together international experts that have been driving this progress to discuss their most recent advancements.

Organized by Christian Carbogno, Saskia Fischer, and Markus Wagner

Time: Wednesday 9:30–13:00 Location: EW 203

**Invited Talk** HL 28.1 Wed 9:30 EW 203

**Green-Kubo lattice dynamics approach to thermal transport in strongly anharmonic materials** — •Ivana Savić — King's College London, UK

Over the last 15 years, there has been a great progress in the development of theoretical and computational tools to describe lattice thermal conductivity in realistic materials from first principles. Standard approaches are based on the phonon Boltzmann transport equation and a perturbative description of phonon-phonon interactions, including only third order anharmonicity. As a result, they are appropriate only for weakly anharmonic materials. In this talk, I will present a new method to simulate lattice thermal transport in strongly anharmonic materials, based on the Green-Kubo formalism and a non-perturbative treatment of phonon-phonon interactions [1]. I will also present the application of this method to understand the lattice thermal conductivity of a well-known thermoelectric material, GeTe, near the ferroelectric phase transition.

[1] D. Dangic, O. Hellman, S. Fahy, and I. Savic, npj Comp. Mater. 7, 57 (2021)

**Invited Talk** HL 28.2 Wed 10:00 EW 203

**Hybrid crystal-glass heat conduction and radiative effects in disordered solids** — •Michele Simoncelli — Theory of Condensed Matter Group of the Cavendish Laboratory, University of Cambridge

At ordinary temperatures, crystals and glasses exhibit opposite thermal conductivities upon heating: decreasing in the former and increasing in the latter. At extreme temperatures, instead, experiments in crystalline and glassy polar dielectrics show a qualitatively similar strong enhancement in their conductivities, which departs from predictions obtained using state-of-the-art heat-conduction theories. Here, we employ and extend the Wigner formulation of thermal transport to shed light on the microscopic physics determining heat transfer in crystals and glasses over a broad temperature range. First, we show that at ordinary temperatures, the magnitude and trend of the conductivity can be engineered through the degree of disorder in the atomistic bond topology, geometry, or composition of a solid, allowing for the emergence of hybrid crystal-glass conductivity trends. Second, we extend the Wigner formulation to account for phonon-photon couplings; relying on such framework, we show from first principles that the conductivity enhancement in polar dielectrics at extreme temperatures originates from an interplay between conductive and radiative heat transfer and is regulated by atomistic disorder.

**Invited Talk** HL 28.3 Wed 10:30 EW 203

**Engineering and probing phonons and thermal transport** — •Ilaria Zardo[1,2], Begoña Abad[1], Chaitanya Arya[1], Giulio de Vito[1], Yashpreet Kaur[1], Dominik M. Koch[1], Grazia Raciti[1], Aswathi K. Sivan[1], Jose M. Sojo[1], and Johannes Trautvetter[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Swiss Nanoscience Institute, University of Basel, Basel, Switzerland

The recently growing research field called "Nanophononics" deals with the investigation and control of vibrations in solids at the nanoscale. Phonon engineering leads to a controlled modification of phonon dispersion, phonon interactions, and transport. However, engineering and probing phonons and phonon transport at the nanoscale is a non-trivial problem.

In this talk, we discuss how phononic properties and thermal transport can be engineered and measured in nanowires and the challenges and progresses in the measurement of the thermal conductivity of nanostructures and low dimensional systems. We experimentally show that a controlled design of the nanowires' phononic properties can be decided à la carte by tuning the superlattice period. We also investigated thermal rectification in semiconducting gallium arsenide nanowires with an abrupt change in diameter, also called telescopic nanowires. We measured rectification values ranging from 2 to 7% at a range of ambient temperatures. Finally, Raman thermometry is used to probe the temperature profile in nanostructures upon application of a thermal gradient, enabling the differentiation between different thermal transport regimes.

**15 min. break**

**Invited Talk** HL 28.4 Wed 11:15 EW 203

**Challenges and opportunities of thermally anisotropic materials** — •Sebastian Reparaz — Materials Science Institute of Barcelona (ICMAB)

The study of the thermal conductivity (or diffusivity) tensor ($\kappa$ij) in bulk and low dimensional materials has gained considerable momentum in recent years. A large number of experimental methods to study the out-of-plane components of the thermal conductivity have been developed and successfully demonstrated using different methodologies, e.g., based on electrical or optical methods. On the other hand, the study of in-plane thermal transport is comparatively more challenging due to the lack of sensitivity to this component of most developed methods, among other reasons. I will discuss two complementary experimental approaches recently developed with enhanced sensitivity to thermal anisotropy and, in particular, to in-plane thermal transport, which are based on using a 1D heat source with uniform power distribution along its long axis. I will show the application of these recently developed methodologies to study the thermal properties of a large variety of samples, with special focus on determining the thermal conductivity tensor elements. In particular, I will address the following list of materials: $\beta$-Ga2O3; highly oriented pyrolytic graphite (HOPG); suspended silicon and polymer membranes with different thicknesses; bismuth, silicon, glass, AlN, GaN, ZnO, and ZnS substrates; and several Van der Waals materials such as PdSe2, hence, demonstrating their excellent performance and rather simple data analysis procedure.

HL 28.5 Wed 11:45 EW 203

**Thermal transient grating, measuring thermal anisotropies on ultra-short length scales** — •Luca Sung-Min Choi[1], Moritz Meissner[1], Alwin Wüthrich[1], Kai Xu[2], Riccardo Mincigrucci[3], Laura Foglia[3], Danny Fainozzi[3], Filippo Bencivenga[3], Sebastian Reparaz[2], and Markus R. Wagner[1,4] — [1]Technische Universität Berlin, Berlin, Germany — [2]Institut de Ciència de Materials de Barcelona, Barcelona, Spain — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Optical transient thermal grating (TTG) is a contactless method to determine anisotropies of thermal transport and acoustic phonons. These physical properties can be observed by fluctuations of the complex diffraction index. Using extreme UV emission of free electron lasers (FELs), ultra-short grating lengths ranging from 110 to 26 nm can be realized. In order to illustrate the possibilities of this method using FELs as emission sources, we exemplary introduce our investigation of the strong anisotropy in the beta-phase of gallium oxide. The experiments were conducted at the Fermi Free Electron Laser [Elettra Synchrotron Trieste, dedicated endstation EIS-TIMER] on a (001)-$\beta - Ga_2O_3$ sample.

HL 28.6 Wed 12:00 EW 203

**Ballistic phonon transport in ß-Ga2O3** — •Rüdiger Mitdank[1], Robin Ahrling[1], Andreas Popp[2], Jana Rehm[2], Arub Akhtar[2], Zbigniew Galazka[2], and Saskia Fischer[1,3] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany — [3]CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

The anisotropic thermal conductivity and the phonon mean free path (mfp) in monoclinic ß-Ga2O3 single crystals and homoepitaxial films of several micron were determined using the 3-$\omega$ method in the temperature range from 10 K-300 K. Analysis of the phonon mfp shows a dominance of phonon-phonon-Umklapp scattering above 80 K, below which the influence of point-defect scattering is observed. Below 30 K the phonon mfp increases and the dominance of boundary effects and the crossover from resistive to ballistic phonon transport is observed. The measured effective thermal conductivity reaches a maximum of 1000-2000 W/(mK) and decreases with T^3 below 25 K. The resistive and ballistic phonon transport regimes in ß-Ga2O3 are discussed corresponding to the models of Callaway (resistive transport - Fourier limit) and Majumdar (phonon radiative transport - Casimir limit), respectively. The Casimir limit is achieved in very pure Ga2O3 single crystals and homoepitaxial layers.

1. A. Majumdar, Journal of Heat Transfer, 115, 7, 1993; 2. Callaway, J, Phys. Rev. 113, 1046, 1959; 3. H. Casimir, Physica, 5, no. 6, 495, 1938

(funded by the DFG: FI932/10-1 and FI932/11-1).

HL 28.7 Wed 12:15 EW 203

**anisotropic thermal conductivity studied with the *ab initio* Green-Kubo approach: the example of $Ga_2O_3$** — •Shuo Zhao, Thomas A. R. Purcell, Kisung Kang, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

Anisotropic heat transport is important in thermoelectric materials and electronic devices since the efficiency of heat dissipation depends on the crystal axis. [1] The anisotropic thermal conductivity is often addressed in the phonon picture, but the role of (strong) anharmonicity is rarely discussed. To clarify this question, we employ the *ab initio* Green-Kubo method, [2] which accounts for all anharmonic effects through *ab initio* molecular dynamics. By extending its applicability to anisotropic transport, we discuss the thermal conductivity for the $\beta$, $\alpha$, and $\kappa$-phase of $Ga_2O_3$, promising candidate materials for field-effect transistors. Our calculations show reasonable agreement with the experiment and allow us to explain the observed anisotropic transport. In particular, we discuss the role of strong anharmonic effects beyond the phonon picture at higher temperatures. In this regard, we also analyze the role of the employed exchange-correlation functional. This study paves the way for exploring the anisotropic, strongly anharmonic systems.

[1] C. Chang *et al.*, *Science* **360**, 778 (2018).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

HL 28.8 Wed 12:30 EW 203

**Computing Green-Kubo Thermal Conductivities with Semi-Local Machine-Learning Potentials** — •Marcel F. Langer[1,2,3,4], Florian Knoop[4,5], J. Thorben Frank[2,3], Christian Carbogno[4], Matthias Scheffler[4], and Matthias Rupp[6] — [1]COSMO Laboratory, EPFL, Lausanne, Switzerland — [2]BIFOLD, Berlin, Germany — [3]ML Group, TU Berlin, Germany — [4]NOMAD Laboratory at the FHI of the Max Planck Society and IRIS Adlershof of HU Berlin, Germany — [5]Theoretical Physics Division, IFM, Linköping University, Sweden — [6]Materials Research and Technology Dept., Luxembourg Institute of Science and Technology, Luxembourg

The Green-Kubo method is a rigorous framework for heat transport simulations in materials, but requires an accurate description of the potential-energy surface and converged statistics. In this context, machine-learning potentials can achieve the accuracy of first-principles methods while allowing to reach well beyond their simulation time and length scales at a fraction of the cost. Recently developed potentials can include equivariant semi-local interactions through message-passing mechanisms and use automatic differentiation to obtain derivatives. We explain how to define and efficiently implement the heat flux for such potentials [1]. Based on this, we present a framework for running GPU-accelerated Green-Kubo calculations with machine-learning potentials, and demonstrate its use through the calculation of the thermal conductivity of several solid semiconductors and insulators.

[1]: M.F. Langer et al., Phys. Rev. B 108, L100302 (2023); M.F. Langer et al., J. Chem. Phys. 159, 174105 (2023)

HL 28.9 Wed 12:45 EW 203

**Quantitatively accurate description of heat transport in metal-organic frameworks** — Sandro Wieser, Florian Lindner, Lukas Legenstein, Lukas Reicht, and •Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Metal-organic frameworks (MOFs) comprise a highly porous class of materials consisting of metal-oxide nodes and organic linkers. They are envisioned for a wide variety of applications, many of which involve the generation or consumption of thermal energy. Therefore, understanding their heat-transport properties is of crucial importance. Unfortunately, MOFs are typically so complex (containing dozens or even hundreds of atoms in their unit cells), that an ab initio-based simulation of thermal transport appears impossible. Also conventional, transferable force fields are not suitable for the task, as they yield thermal conductivity values far from experiments. In the current contribution we show that the situation can be resolved employing on-the-fly-trained, machine-learned potentials (MLPs), which enable an essentially ab initio-quality description of phonon properties of MOFs at computational costs reduced by many orders of magnitude. Interestingly, with accurate MLPs at hand, various applied methodologies (NEMD, AEMD, Green-Kubo MD, as well as lattice dynamics) yield equivalent results in quantitative agreement with experimental, single crystal data. A similar situation is encountered for polymers and molecular crystals. The results pave the way for a reliable, atomistic understanding of heat transport in the said materials.

# HL 29: Quantum Transport and Quantum Hall Effects

Time: Wednesday 9:30–12:00 Location: EW 561

**Invited Talk** HL 29.1 Wed 9:30 EW 561

**Nonreciprocal charge transport on the edges of a quantum anomalous Hall insulator** — •Gertjan Lippertz[1,2], Anjana Uday[1], Andrea Bliesener[1], Lino Pereira[2], Alexey Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Cologne, Germany — [2]Quantum Solid State Physics, KU Leuven, Leuven, Belgium

The quantum anomalous Hall insulator (QAHI) is characterized by a zero longitudinal resistivity and a quantized Hall resistance without the need of an external magnetic field. However, when reducing the device dimensions or increasing the current density, an abrupt breakdown of the dissipationless state occurs. We have previously proposed that this breakdown originates from the electric-field-driven percolation of charge puddles in the 2D bulk states of the compensated thin film [1]. It was recently reported that the interplay between the 1D chiral edge state and the 2D bulk states in a QAHI can give rise to nonreciprocal charge transport [2]. So far, this nonreciprocity was only studied in the broken-down QAHI state at elevated temperatures and at high excitation currents [2], and hence its emergence from the low-current, dissipationless regime remains to be understood. In this talk, we show that the onset of 2D bulk conduction due to breakdown is sufficient to create the nonreciprocal effect, and interestingly, there is a sign change in the nonreciprocity with increasing current, suggesting a crossover in the underlying mechanism of the nonreciprocal transport.

[1] Lippertz et al., Phys. Rev. B 106, 045419 (2022)
[2] Yasuda et al., Nat. Nanotechnol. 15, 831-835 (2020)

HL 29.2 Wed 10:00 EW 561

**Visualizing electronic transport in the quantum anomalous Hall regime** — •George Ferguson[1], Run Xiao[2], Anthony Richardella[2], Nitin Samarth[2], and Katja Nowack[1] — [1]Laboratory of Atomic and Solid-State Physics, Cornell University — [2]Department of Physics, The Pennsylvania State University

We report a magnetic imaging study of the current distribution in the quantum anomalous Hall regime. We use a scanning superconducting quantum interference device (SQUID) microscope with micrometer scale spatial resolution to image the magnetic fields above Cr-doped (Bi,Sb)2Te3 samples. From these data we reconstruct the local current density, allowing us to visualize the current distribution in our devices. We find that most current flows in the bulk when the transport coefficients are quantized. By combining this observation with images of the equilibrium magnetization, we construct a comprehensive picture of electronic transport in the quantum anomalous Hall regime.

HL 29.3 Wed 10:15 EW 561

**Microwave transport in quantum anomalous Hall edge states** — •Torsten Röper, Hugo Thomas, Daniel Rosenbach, Christian Dickel, Anjana Uday, Gertjan Lippertz, Alexey Taskin, Yoichi Ando, and Erwann Bocquillon — Physics Institute II, University of Cologne, Cologne, Germany

Magnetically doped topological insulators such as V-doped $(Bi_xSb_{1-x})_2Te_3$ (V-BST) show the quantum anomalous Hall (QAH) effect. These materials exhibit a quantized Hall conductance without an applied external magnetic field, owing to the presence of a non-zero Chern number. A single chiral edge state emerges at the edge of the QAH material and is topologically protected against disorder and perturbations. Microwave transport in chiral edge states allows for investigating the dispersion and velocity of the edge states.

In this context, we conduct microwave measurements on devices using V-BST films grown by molecular beam epitaxy. We measure the transmission of the edge states as a function of temperature, magnetic field and frequency. We determine their velocity and attenuation from the phase and amplitude, respectively. Following recent works, we ascribe the interaction with charge puddles as a primary source of dissipation. We describe this interaction with a circuit model and observe a dispersion consistent with findings in similar materials. As such, it provides a potential material platform for coherent electronic transport in chiral edge states and the generation and manipulation of flying Majorana excitations.

HL 29.4 Wed 10:30 EW 561

**Anomalous conductance steps in 3DTI HgTe-based QPCs** — •Elisabeth Richter[1], Michael Barth[2], Dmitriy Kozlov[1], Juliane Steidl[1], Klaus Richter[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

Previously, 3DTI strained HgTe-based nanowires were studied in an axial magnetic field, exhibiting Aharonov-Bohm type oscillations [1]. Here, we study the conductance of short QPCs of different width and height in a perpendicular magnetic field. The QPCs are fabricated by lithography and etching, resulting in ballistic but non-adiabatic transport. Zero-field gate voltage traces show no quantisation and conductance in the range of 1 to 100 $e^2/h$. In a quantising magnetic field, pronounced conductance plateaus are observed, coinciding with the position of the integer filling factors of the macroscopic part of the sample. Surprisingly, for narrow QPCs, the values of the plateaus are smaller than expected for the corresponding filling factors. Such behaviour could be considered as trivial impurity scattering; however, we found that certain conductance values are preferred over others. We hypothesise that the QPC acts as a kind of filter whose transmission depends on the structure of the energy bands in the QPC.

[1] Ziegler, J. et al., Phys. Rev. B 97, 035157 (2018)

**15 min. break**

HL 29.5 Wed 11:00 EW 561

**Spin splitting and disorder of Landau levels in HgTe-based Dirac fermions** — •Dmitriy Kozlov, Johannes Ziegler, and Dieter Weiss — Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany

This study conducts experimental exploration into a system of two-dimensional Dirac fermions, utilizing a critical thickness HgTe quantum well in weak magnetic fields. The formation and evolution of Shubnikov-de Haas (SdH) oscillations in the magnetotransport and the capacitive response are studied, complemented by calculations of Landau levels (LLs). It is shown that the behavior of the LLs is influenced not only by the linear dispersion law of the carriers and the Zeeman splitting, but also by the splitting of the Dirac cones in zero magnetic field caused by interface inversion asymmetry (IIA). The measured value of the splitting is 1.5 meV. The behavior of the zero LL is studied and its spin splitting is demonstrated. It is shown that the broadening of the zero LL is several times higher than that of the other levels due to the lack of charge impurity screening.

HL 29.6 Wed 11:15 EW 561

**In-plane electric-field effects at transitions between quantum Hall plateaus in InAs-based quantum wells** — •Olivio Chiatti[1], Johannes Boy[1], Christian Heyn[3], Wolfgang Hansen[3], and Saskia F. Fischer[1,2] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg, 20148 Hamburg, Germany

The cross-over from quasi-two- to quasi-one-dimensional electron transport is studied in dependence of transverse electric fields and perpendicular magnetic fields, both in the diffusive to quasi-ballistic and in the zero-field to quantum Hall regime. Hall-bars and in-plane gates have been fabricated from an InGaAs/InAlAs/InAs quantum well hosting a 2DEG. Magnetotransport measurements at temperatures down to 50 mK and fields up to 12 T show a high effective Lande-factor of $|g^*| = 16$, allowing to resolve spin-split subbands at magnetic fields of 2.5 T. In the quantum Hall regime, electrostatic change of the effective constriction width enables control of the reflection and transmission of edge channels, allowing to separate fully spin-polarized edge channels at filling factors $\nu = 1$ und $\nu = 2$. A change in the orientation of a transverse in-plane electric field in the constriction shifts the transition between Zeeman-split quantum Hall plateaus by $\Delta B \approx 0.1$ T and is consistent with an effective magnetic field of $B_{eff} \approx 0.13$ T by spin-dependent backscattering, indicating a change in the spin-split density of states.

HL 29.7 Wed 11:30 EW 561

**Topological band structure of InAs/GaSb/InAs and**

**InAs/GaInSb/InAs triple quantum wells** — •Sebastian Gebert — Technische Physik, Physikalisches Institut, Am Hubland, D-97074 Würzburg, Germany

Going back to the initial proposal of Kane and Mele [1], the 2D topological insulator (TI) has attracted considerable attention. The first experimental demonstrations of such a TI phase were obtained in HgCdTe/HgTe/HgCdTe and InAs/GaSb quantum wells (QWs). In both cases the TI phase was restricted to cryogenic temperatures either by the strong temperature dependence of the bands or the inherently small bulk bandgap. A promising approach to overcome these limitations was proposed by Ref. [2]. They theoretically demonstrated, that by modifying the known InAs/GaSb QWs with an additional layer it is possible to realize a plethora of different phases, including a TI phase. More precisely, an InAs/GaSb/InAs TI could reach a bulk bandgap of 16 meV and a strained InAs/GaInSb/InAs TI up to 60mV. We here present gate voltage and temperature dependent magnetotransport measurements of InAs/GaSb/InAs and InAs/GaInSb/InAs QWs grown primarily in the TI phase. For later ones, we extract a bulk bandgap of 45 meV and the occuring edge conductivity, which persists up to 40 K, is attributed to the topological edge channels.

[1] C. L. Kane & E. J. Mele, Phys. Rev. Lett. 95, 146802
[2] S. S. Krishtopenko & F. Teppe, Science Advances Vol. 4, NO. 4
[3] C. Avogadri et al., Phys. Rev. Research 4, L042042

HL 29.8 Wed 11:45 EW 561

**Giant Negative Magnetoresistance as a Function of the Electron Density** — •Lina Bockhorn[1], Dieter Schuh[2], Christian Reichl[3], Werner Wegscheider[3], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [3]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases not only show an increasing number of new fractional filling factors, but also an astonishing robust negative magnetoresistance at zero magnetic field [1 -4]. In-situ variation of the electron density enables a deep insight into the nature of the negative magnetoresistance. Here, we investigate the temperature-dependent giant negative magnetoresistance (GNMR) as a function of the electron density for several temperatures and currents. For low densities, the temperature dependence of the GNMR is described by the electron-electron interaction correction to the conductivity considering mixed disorder [5]. In the case of higher electron densities, a non-linear current dependence is observed which has to be described within the hydrodynamic regime [6].

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] A. T. Hatke et al., Phys. Rev. B 85, 081304 (2012).
[3] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[4] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[5] I. V. Gornyi et al., Phys. Rev. B. 69, 045313 (2004).
[6] P. S. Alekseev, Phys. Rev. Lett. 117, 166601, (2016).

## HL 30: Ultrafast Phenomena II

Time: Wednesday 10:00–12:15 Location: EW 015

HL 30.1 Wed 10:00 EW 015

**Ultrafast coherent exciton dynamics and manybody interactions in a WS2 monolayer** — Daniel Timmer[1], •Moritz Gittinger[1], Daniel Lünemann[1], Sven Stephan[1,2], Martin Silies[1,2], Antonietta De Sio[1], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]University of Applied Sciences Emden, Germany

Monolayers of transition metal dichalcogenides (TMDCs) are quantum materials with fascinating optoelectronic properties. In particular, valleytronic applications are exploiting the spin-selectivity that is provided by the valley pseudospin and large energy splitting between A and B excitons due to strong spin-orbit coupling. However, manybody interactions lead to rapid valley depolarization. In particular, exchange interactions lead to a mixing of A and B excitons. We use ultrafast pump-probe and two-dimensional electronic spectroscopy (2DES), the ideal tool to investigate coherent couplings and manybody interactions in semiconductors, to directly probe these A-B exciton interactions in a monolayer of WS2. We observe the signatures of coherent couplings between the A and B excitons, cross-peaks in the 2DES maps. The associated coherent Rabi oscillations with ˜11.5-fs period are also resolved. In addition, the 2DES data gives detailed insight into the formation of manybody interactions on a tens of fs timescale. The observed coherent couplings are likely reflecting a Dexter-type intervalley exchange interaction. Broadband ultrafast spectroscopy with sufficiently high time-resolution proofs therefore essential in directly probing the coherent quantum dynamics in the time domain.

HL 30.2 Wed 10:15 EW 015

**Ultrafast phonon-driven exciton Rabi oscillations in halide perovskites** — X.Trung Nguyen[1], Katrin Winte[1], Daniel Timmer[1], Yevgeny Rakita[2], Sufyan Ramzam[1], Caterina Cocchi[1], Michael Lorke[3], Frank Jahnke[3], David Cahen[2], Christoph Lienau[1], and •Antonietta De Sio[1] — [1]Universität Oldenburg — [2]Weizmann Institute of Science — [3]Universität Bremen

Coupling electromagnetic radiation with matter is highly promising for tailoring optoelectronic properties and photoinduced dynamics of functional materials. Here we show that even the internal fields induced by coherent lattice motions can transiently control the ultrafast excitonic response in halide perovskites(HaPs). Temperature-dependent ultrafast two-dimensional electronic spectroscopy reveals that the characteristic low-frequency phonons of the soft lead-halide lattice induce strong mixing of 1s and 2p exciton manifolds in $CsPbBr_3$ and $MAPbBr_3$. This results in side-peaks in the spectra and 100-fs-Rabi oscillations in the dynamics. The temperature-dependence of the Rabi oscillations provides insight into dephasing mechanisms within the excited exciton manifold. Our results show that the conventional Fröhlich model is insufficient to describe the behavior of these materials. Instead, they indicate the importance of nonadiabatic couplings. An important implication is that intrinsic optical phonon fields in HaPs may be exploited to transiently modify their optoelectronic properties, and to explore fundamental field-matter interactions toward shaping coherent exciton dynamics by strong and ultrastrong coupling to phonons.

HL 30.3 Wed 10:30 EW 015

**Transient core-hole screening investigated by time-resolved X-ray absorption spectroscopy at the Zn K-edge of ZnO** — •Thomas C. Rossi[1], Lu Qiao[2], Keith Gilmore[2], Ronaldo Rodrigues Pelà[2], Claudia Draxl[2], and Renske M. van der Veen[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [2]Department Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Understanding the ultrafast electronic and lattice response of photoexcited semiconductor materials at the atomic level is crucial for the realization and optimization of devices. Here, we report on the picosecond dynamics of atoms and photoexcited charge carriers above the optical band gap of ZnO in oriented nanorods and thin films by time-resolved X-ray absorption spectroscopy (TRXAS) at the Zn K-edge. The transient signal reveals the non-local screening of the core-hole potential by photogenerated electron-hole pairs, often overlooked in previous studies on photoexcited semiconductors. State-of-the-art calculations with the Bethe Salpeter equation are able to reproduce the spectral features and the non-linear effect of the core-hole screening on the transient with the excitation density. Theoretical predictions are made on the effect of the pump/probe polarization and efficiency of the non-local screening on the femtosecond timescale. This work highlights the simultaneous sensitivity of TRXAS to incoherent atomic motions and delocalized photoexcited carriers with chemical element sensitivity, which opens new perspectives for the study of photoexcited semiconductors in complex materials or in optoelectronic devices.

HL 30.4 Wed 10:45 EW 015

**Lightwave-control of on-chip femtosecond electronics** — •Johannes Schmuck[1,2], Johannes Gröbmeyer[1,2], Maximilian Auers[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 Technolgy (MCQST), Munich, Germany

Ultrashort laser pulses allow the generation of light-driven electrical

currents [1]. By different photoemission processes the generation of THz electric pulses on on-chip circuits is possible. The corresponding pulses with increased bandwidths up to 10 THz can propagate along macroscopic striplines on a millimeter scale [2]. Rather than using femtosecond photoswitches based on photoconductivity or biased tunneling barriers in nanoscale metal junctions to drive the pulses [3], we investigate direct control of the electronic pulses by single-cycle laser pulses.

[1] M. Ludwig et al. Sub-femtosecond electron transport in a nanoscale gap. Nat. Phys. 16, 341-345 (2020). [2] C. Karnetzky et al. Towards femtosecond on-chip electronics based on plasmonic hot electron nano-emitters. Nat Commun 9, 2471 (2018). [3] J. Gröbmeyer et al. Space-charge limited and ultrafast dynamics in graphene based nano-gaps. Appl. Phys. Lett. 123, 013504 (2023).

**15 min. break**

HL 30.5 Wed 11:15 EW 015

**Full calculation of the observable for HHG in solids** — •Francisco Navarrete and Dieter Bauer — Institute of Physics, University of Rostock, 18051 Rostock, Germany

When an intense infrared laser interacts with a target, it can produce radiation at frequencies that are multiples of the central frequency of the driving source. This is known as high-harmonic generation (HHG), which was first investigated for atomic and molecular targets [1] and later for condensed matter [2]. The growing attention to explain the impact of the quantum nature of the driving pulse [3], along with the recognized discrepancies between the spectra in HHG in solids obtained from numerical calculations and experiments [4], has encouraged the pursuit of new methods to compute the spectra [5]. In this study, we demonstrate the distinctions in the harmonic spectrum of HHG in solids by comparing the conventional calculation method of the observable [6] with an alternative approach that takes into account typically overlooked terms. Additionally, we examine the underlying physics behind these dissimilarities. [1] M. Lewenstein et al., Phys. Rev. A 49, 2117 (1994) [2] S. Ghimire et al., Nat. Phys. 7, 138 (2011) [3] M. Lewenstein et al., Nat. Phys. 17, 1104 (2021) [4] I. Floss et al., Phys. Rev. A 97, 011401(R) (2018). [5] A. Gorlach et al., Nat Commun 11, 4598 (2020) [6] B. Sundaram and P. W. Milonni, Phys. Rev. A 41, 6571(R) (1990)

HL 30.6 Wed 11:30 EW 015

**Modelling dephasing effects in High Harmonic Generation in a real space Tight-Binding-approach** — •Martin Thümmler[1], Alexander Croy[1], Ulf Peschel[2], and Stefanie Gräfe[1] — [1]Institute of Physical Chemistry, University of Jena — [2]Institute of Condensed Matter Theory and Optics, University of Jena

High harmonic generation in bulk materials is commonly described by semiconductor Bloch equations employing ultrashort dephasing times ($\sim$ 2 fs). Those are chosen to match the clear harmonic peaks observed in experiments, but contradict spectroscopic measurements of narrow linewidth excitonic peaks in semiconductors. Therefore the physical origin of these short dephasing times is currently strongly debated.

In this talk, we focus on real space dephasing models starting from our periodic real space Tight-Binding model. Extending this model, we discuss the effect of different real space dephasing mechanisms on the calculated high harmonic spectra.

HL 30.7 Wed 11:45 EW 015

**Time-resolved on-chip electronics in the THz regime** — Johannes Schmuck[1,2], •Maximilian Auers[1,2], Johannes Gröbmeyer[1,2], Nina Pettinger[1,2], Sergey Zherebtsov[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]MCQST

Our study explores on-chip circuits driven by ultrashort femtosecond pulses, which allow an increased bandwidth of up to 10 THz [1]. The circuits employ macroscopic striplines spanning on the micrometer scale to facilitate the propagation of corresponding electronic pulses. We present a two-temperature heat model investigating the heat dissipation across the metal electrodes in combination with different substrate materials. Such stripline circuits mark a pivotal advancement toward the integration of femtosecond electronics within on-chip quantum circuits.

[1] C. Karnetzky et al. Towards femtosecond on-chip electronics based on plasmonic hot electron nano-emitters. Nat Commun 9, 2471 (2018).

HL 30.8 Wed 12:00 EW 015

**First-Order Rhombohedral to Cubic Phase Transition in Photoexcited GeTe** — •Matteo Furci, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Photoexcited GeTe undergoes a non-thermal phase transition from a rhombohedral to a rocksalt crystalline phase. The microscopic mechanism and the nature of the transition are unclear. By using constrained density functional perturbation theory and by accounting for quantum anharmonicity within the stochastic self-consistent harmonic approximation, we show that the non-thermal phase transition is strongly first order and does not involve phonon softening, at odd with the thermal one. The transition is driven by the closure of the single particle gap in the photoexcited rhombohedral phase. Finally, our work shows how ultrafast XRD data are consistent with a coexistence of the two phases, as expected in a first order transition. Our results are relevant for the understanding of phase transitions and bonding in phase change materials.

## HL 31: Focus Session: Evolution of Topological Materials into Superconducting Nanodevices II (joint session HL/TT)

The focus session intends to span the arc between topological materials and superconducting nanodevices, both experimentally and theoretically. Such structures are interesting for applications in future topological quantum circuits. In recent years, the number of topological materials and the knowledge about them has rapidly increased. As part of the focus session, material properties of layered systems made of topological materials, especially in combination with superconductors, are discussed. On the other hand, the special challenges in the nanofabrication of these materials for use in future topological quantum processors are addressed. Another focus is the quantum transport in nanoscale hybrid structures.

Organized by Thomas Schäpers, Philipp Rüßmann, and Peter Schüffelgen

Time: Wednesday 11:45–13:00 Location: EW 202

HL 31.1 Wed 11:45 EW 202

**Induced superconducting correlations in the quantum anomalous Hall insulator** — •Anjana Uday[1], Gertjan Lippertz[1,2], Kristof Moors[3], Henry F. Legg[4], Rikkie Joris[2], Andrea Bliesener[1], Lino M. C. Pereira[2], Alexey Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Köln, Germany — [2]KU Leuven, Quantum Solid State Physics, Leuven, Belgium — [3]Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, Jülich, Germany — [4]Department of Physics, University of Basel, Basel, Switzerland

Crossed Andreev reflection (CAR) has been reported in a hybrid quantum Hall (QH)/Superconductor (SC) system [1]. Similar experiments would be of great interest for quantum anomalous Hall (QAH) systems. It has been predicted that if Cooper pairing is induced in a QAH insulator, the system turns into a stereotypical spinless chiral

p-wave superconductor associated with chiral Majorana edge states. In the QAH/SC system superconductivity can be suppressed by applying a magnetic field while keeping the 1D chiral edge state intact. Here we report the observation of crossed Andreev reflection (CAR) across a narrow superconducting Nb electrode contacting the chiral edge state of a QAHI, evinced by a negative nonlocal voltage measured downstream from the grounded Nb electrode. By changing the Nb width, the characteristic length of the CAR process is identified to be about 100 nm, which is three times longer than the superconducting correlation length in Nb.

[1] Lee et al., Nat. Phys., 13 (2017) 693-698

HL 31.2 Wed 12:00 EW 202

**Work function engineering in superconducting Ir/Nb(110) films** — •Adamantia Kosma[1], Stefan Blügel[1], and Philipp Rüssmann[1,2] — [1]Forschungszentrum Jülich — [2]University of Würzburg

The topological superconducting hybrid structures have been attracting considerable research interest in recent years, as they are promising candidates for topologically protected qubits. Because of this, a substantial demand for appropriate superconducting substrates has been created. In our study we explore the superconducting properties of Ir/Nb(110) films. Our focus is on the investigation of the change in the work function and the size of the proximity-induced superconducting gap of Ir overlayers deposited on Nb(110). The work function plays a crucial role in determining the behavior of electrons at the superconducting surface, thereby influencing the charge transport. In the specific context of superconductor hybrid structures for Majoranas, the target is to effectively manage the work function mismatch while maintaining a robust proximity effect through the overlayer. This approach will also provide valuable information for studying the proximity effect in a topological insulator/superconductor(TI/SC) system. Our findings are based on first-principles calculations using the full-potential Korringa-Kohn-Rostoker Green function method and its Kohn-Sham Bogoliubov-de Gennes (KS-BdG) extension to describe superconducting heterostructures [1].

We thank the ML4Q (EXC 2004/1 - 390534769) for funding.

[1] P. Rüßmann, and S. Blügel, Phys. Rev. B **105**, 125143 (2022).

HL 31.3 Wed 12:15 EW 202

**Superconducting transition metal dichalcogenites for TI-based topological superconducting devices** — •Philipp Rüssmann — Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

Proximitized topological insulators (TIs) are promising materials to build topological superconductors with the promise to realise Majorana-zero modes and topologically protected quantum devices. Here, we present an overview over our recent computational studies of heterostructures between superconducting transition-metal dichalcogenites (TMDCs) and TIs [1,2]. We compare different TMDC/TI interfaces and analyze the influence of the TMDCs on charge doping, band alignment and the superconducting proximity effect in the TI.

In our work we employ Kohn-Sham Bogoliubov-de Gennes simulations for the superconducting electronic structure based on density functional theory which is implemented in the full-potential relativistic Korringa-Kohn-Rostoker Green function method [3,4].

[1] Xian-Kui Wei *et al.*, arXiv 2311.16590 (2023)
[2] Abdur Rehman Jalil *et al.*, in preparation (2023)
[3] P Rüßmann and S Blügel, PRB **105**, 125143 (2022).
[4] JuDFTteam/JuKKR (2022). doi: 10.5281/zenodo.7284738

HL 31.4 Wed 12:30 EW 202

**Superconducting diode effect in topological insulator nanowire Josephson junctions** — •Ella N. Nikodem, Jakob Schluck, Mahasweta Bagchi, Zhiwei Wang, and Yoichi Ando — Physics Institute II, University of Cologne, Zülpicher Straße 77, 50937 Köln, Germany

Topological insulator nanowires coupled to conventional superconductors were predicted to host Majorana zero modes more than a decade ago [1]. An indication of the presence of such Majorana bound states in Josephson junction devices based on these nanowires is an enhanced superconducting diode effect in the topological regime, attributed to their $4\pi$-periodic contribution to the current phase relation [2]. In this talk, we report our investigations of the superconducting diode effect in side-contacted etched nanowires made from exfoliated flakes of the bulk-insulating topological insulator BiSbTeSe2. We observed a strong dependence of the critical current on gate voltage and the magnetic field along the nanowire, as well as a significant superconducting diode effect. Its direction and magnitude can be switched by tuning the aforementioned parameters. Possible relevance of the Majorana bound states in the observed diode effect will be discussed.

[1] A. Cook and M. Franz, Phys. Rev. B 84, 201105(R) (2011).
[2] H. F. Legg et al., arXiv:2301.13740 (2023).

HL 31.5 Wed 12:45 EW 202

**Nanoscale patterning of topological insulator thin film using a helium ion microscope** — •Holger Mirkes[1,2], Filippo Romano[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institute and Physik-Department, Technical University of Munich, Germany. — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany.

The helium ion microscope has evolved as a versatile tool for not only nanoscale imaging, but also nanoscale fabrication with a resolution well below 10 nm, limited only by substrate proximity effects for atomically thin films [1]. Here, we discuss the application of He-ion beam milling for nanofabrication of lateral superlattice structures in topological insulator thin films. We present results both on supported films grown by molecular beam epitaxy as well as on suspended films prepared by scotch tape exfoliation. The superior resolution of the He-ion microscope may be used to create lateral superlattice structures with topologically protected satellite Dirac cones [2]. The research is supported through the European Union*s Horizon Europe Research and Innovation Programme under Grant Agreement No 101076915 (2DTopS).

[1] E. Mitterreiter et al., Nano Lett. 2020, 20, 4437*4444.
[2] J. Cano et al., Phys. Rev. B 2021, 103, 155157.

# HL 32: Spin Phenomena in Semiconductors

Time: Wednesday 15:00–16:15 Location: EW 015

HL 32.1 Wed 15:00 EW 015

**Hole spin coherence in InAs/InAlGaAs self-assembled quantum dots emitting at telecom wavelengths.** — Eiko Evers[1], Natalia Kopteva[1], •Vitalie Nedelea[1], A Kors[2], Ranbir Kaur[2], Johann Reithmaier[2], Mohamed Benyoucef[2], Manfred Bayer[1], and Alex Greilich[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, D-34132 Kassel, Germany

We report measurements of the longitudinal and transverse spin relaxation times of holes in an ensemble of self-assembled InAs/InAlGaAs quantum dots (QDs) emitting in the telecom spectral range. The spin coherence of a single carrier is determined by spin mode locking in the inhomogeneous ensemble of QDs. By modelling the signal, the hole spin coherence time can be extracted to be in the range of T2 = 0.02 - 0.4 *s. The longitudinal spin relaxation time T1 = 0.5 *s is measured by the spin inertia method. Using the spin mode-locking method, we could deter mine the range of the achievable spin coherence of holes, which exceed previously measured values in similar types of QDs by at least an order of magnitude. The longitudinal spin lifetime of 0.5 $\mu$s is also extended and currently provides the upper limit for the spin coherence.

HL 32.2 Wed 15:15 EW 015

**Long-Range Proximity Effect in Magnetite Hybrid Ferromagnet-Semiconductor** — Ina Kalitukha[1,2], •Eyüp Yalcin[1], Olga Ken[1,2], Vladimir Korenev[1,2], Ilya Akimov[1,2], Carolin Harkort[1], Grigorii Dimitriev[2], Dennis Kudlacik[1], Victor Sapega[2], Vitalie Nedelea[1], Evgeny Zhukov[1,2], Dmitri Yakovlev[1,2], Al Banshchikov[2], Andrey Kaveev[2,3], Grzegorz Karczewski[4], Tomasz Wojtowicz[5], Martina Müller[6], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]St. Petersburg, Russia — [3]St. Petersburg, Russia — [4]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [5]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [6]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We studied long-range proximity effect in hybrid ferromagnet-semiconductor structure between the ferromagnetic (FM) semimetal magnetite ($Fe_3O_4$) layer and CdTe quantum well (QW) using time-integrated and time-resolved photoluminescence (PL) spectroscopy techniques. The magnetite FM layer and a CdTe QW are separated by a 10 nm thick (Cd,Mg)Te barrier. The proximity effect is manifested in the circularly polarized photoluminescence corresponding to the recombination of photoexcited electrons with holes bound to shallow acceptors in the QW induced by the FM layer.

HL 32.3 Wed 15:30 EW 015

**Extended Spin Lifetimes in Transition Metal Doped Hybrid Lead Halide Perovskites** — •Jonathan Zerhoch[1,2,3], Stanislav Bodnar[1], Jamie Lerpiniere[4], Shangpu Liu[1,2,3], Timo Neumann[2,3,5], Barbara Sergl[2,3], Markus W. Heindl[1,2,3], Andrii Shcherbakov[1,2,3], Ahmed Elghandour[6], Rüdiger Klingeler[6], Alison Walker[4], and Felix Deschler[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Walter Schottky Institut, Technische Universität München — [3]Physics Department, TUM School of Natural Sciences, Technische Universität München — [4]Department of Physics, University of Bath — [5]Cavendish Laboratory, University of Cambridge — [6]Kirchhoff Institut für Physik, Universität Heidelberg

The outstanding optoelectronic properties of hybrid metal halide perovskites, and their strong spin-orbit coupling, enable efficient manipulation of the charge carrier's angular momentum. In this work, we investigate the dominant spin relaxation mechanism in $CH_3NH_3PbBr_3$ polycrystalline thin films with nominal doping levels up to 50% with the transition metal $Mn^{2+}$ . We investigate the spin relaxation times in these paramagnetic hybrid semiconductors with ultrafast circularly polarized broadband transient absorption spectroscopy at cryogenic temperatures. Using quantitative theoretical analysis of the photoexcitation cooling processes, we identify increased carrier momentum scattering rates extending the spin relaxation lifetimes by a factor of three. We explain this observation with motional narrowing effects in the paramagnetic ensemble of $Mn^{2+}$ impurities.

HL 32.4 Wed 15:45 EW 015

**Extension of the coherent optical response from the trions localized in InGaAs quantum dots** — •Alexander Kosarev[1,2], Artur Trifonov[2,3], Irina Yugova[3], Iskander Yanibekov[3], Sergey Poltavtsev[2,3], Aleksandr Kamenskii[2], Sven Scholz[4], Carlo Alberto Sgroi[4], Arne Ludwig[4], Andreas Wieck[4], Dmitri Yakovlev[2], Manfred Bayer[2], and Ilya Akimov[2] — [1]Technical University Berlin, Germany — [2]Technical University Dortmund, Germany — [3]St. Petersburg, Russia — [4]Ruhr-University Bochum, Germany

A sequence of optical pulses can store the optical fields in the ensemble of quantum emitters and subsequently retrieve them in the form of photon echoes (PE). The limiting factor for such storage is the decoherence time of the quantum emitter, which can be extended by transferring the coherence from the emitter to its spin degrees of freedom, which was earlier seen in bulk material and quantum wells. In the work, we report such an extension of the coherent response by an order of magnitude to 4 ns, observed on the negatively charged InGaAs self-assembled quantum dots using three-pulse spin-dependent PE in the moderate transverse magnetic field. We revealed that the non-zero transverse hole g-factor must be accounted in the temporal evolution of such systems because of its strong impact on the long-lived PE signal. Thus, transfer of the coherence from the emitter to the optical degrees of freedom with a subsequent retrieval was first observed in ensembles of the quantum dots, non-zero transverse hole g-factor was accounted in the existing model to describe evolution of such system.

HL 32.5 Wed 16:00 EW 015

**Magnetic transparent conductors for spintronics** — •Pino D'Amico[1], Alessandra Catellani[1], Alice Ruini[2], Stefano Curtarolo[3], Marco Fornari[4], Marco Buongiorno Nardelli[5], and Arrigo Calzolari[1] — [1]Istituto Nanoscienze CNR-NANO-S3, I-4115 Modena, Italy — [2]Dipartimento FIM Universitá di Modena e Reggio Emilia, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, Duke University, Durham, NC 27708, USA — [4]Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859 — [5]Department of Physics, University of North Texas, Denton, TX 76203, USA

Transparent Conductors (TCs) exhibit optical transparency and electron conductivity, and are essential for many opto-electronic and photo-voltaic devices. The most common TCs are electron-doped oxides, which have few limitations when transition metals are used as dopants. Non-oxides TCs have the potential of extending the class of materials to the magnetic realm, bypass technological bottlenecks, and bring TCs to the field of spintronics. In this contribution we propose new functional materials that combine transparency and conductivity with magnetic spin polarization that can be used for spintronic applications, such as spin filters. By using high-throughput first-principles techniques, we identified a large number of potential TCs, including non-oxides materials. Our results indicate that proper doping with transition metals introduces a finite magnetization that can provide spin filtering up to 90% in the electrical conductivity, still maintaining a transparency greater than 90%.

# HL 33: 2D Materials and Heterostructures: Optoelectronics

Time: Wednesday 15:00–16:15 Location: EW 201

HL 33.1 Wed 15:00 EW 201

**Surface acoustic wave-controlled photocurrent in few-layer WSe2** — •Benjamin Mayer, Clemens Strobl, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

The unique combination of piezo-electric surface acoustic waves (SAWs), high-resolution optical spectroscopy and electrical transport provides a versatile testbed to sense and manipulate the optical properties and carrier transport processes in novel nanoscale materials and opens pathways to novel acousto-optoelectronic devices [1]. Here, we present the fabrication and validation of a hybrid platform comprising strong SAW-devices on piezoelectric LiNbO3 and mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials. In our experiments, we employ the SAWs dynamic electric field with a frequency of 150-250MHz to induce a SAW power dependent Acousto-Electric Current (AEC) in few-layer WSe2 placed on top of two gold electrodes. The SAW directional dependence of this fundamental effect enables a detailed investigation of the Au-TMDC interface. Furthermore, the TMDC can be photodoped via excitation with a green laser (532nm) to deeply study the underlying charge carrier dynamics. In the low SAW-Power regime photogating leads to an enhanced AEC by two orders of magnitude, whereas bipolar charge carrier transport sets in for higher SAW powers. [1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 33.2 Wed 15:15 EW 201

**Strong field valleytronics in bulk MoS2** — •Igor Tyulnev[1], Álvaro Jiménez-Galán[2], Julita Poborska[1], Lenard Vamos[1], Rui F. Silva[3], Philip St. J. Russell[4,5], Francesco Tani[4], Olga Smirnova[2,6], Misha Ivanov[2,7,8], and Jens Biegert[1,9] — [1]ICFO, Barcelona, Spain — [2]MBI, Berlin, Germany — [3]ICMM, Madrid, Spain — [4]MPL, Erlangen, Germany — [5]FAU, Erlangen, Germany — [6]TU, Berlin, Germany — [7]HU, Berlin, Germany — [8]Imperial College, United Kingdom — [9]ICREA, Barcelona, Spain

Light field control over condensed matter allows the tailoring of material properties and exploits topology with which classical and quantum operations can be realized in next-generation devices. At this forefront are valleytronics which exploit the valley degree of freedom to provide an optical switch between extrema in the band structure. Resonant excitation distinguishes these valleys through selection rules derived from symmetry breaking of time inversion by circular polarized light fields and of space inversion in monolayer materials. Thus, requiring not only specific excitation wavelengths but also limiting possible material platforms. In this work, we, for the first time, validate a novel, off-resonant approach to valley control based on the synthesis of a bicircular field which by symmetry matching 2H-MoS2 controls the band structure. We demonstrate that strong-field valley control is possible, universal and, at optical speeds, unlocks a path towards engineering efficient, multilayer devices operating on sub-optical cycle timescales.

HL 33.3 Wed 15:30 EW 201

**Near field photocurrent nanoscopy at a biased graphene interface junction** — •Francesca Falorsi[1], Marco Dembecki[2], Christian Eckel[1], Monica Kolek Martinez de Azagra[1], and R. Thomas Weitz[1] — [1]1st Institute of Physics, Faculty of Physics, Georg-August-University Göttingen, Göttingen — [2]Physics of Nanosystems, Faculty of Physics, LMU Munich, Germany; current address. WSI, TUM, Garching, Germany

The nanoscale analysis of photocurrent is a versatile tool to gain information about electronic states, quantum processes, and device characteristics of quantum materials. When photocurrent is studied with a near-field scattering microscope (s-SNOM), it is possible to overcome the diffraction limit. Thus one can image the local characteristic of the devices with a 20 nm resolution. In this work, the analysis of s-SNOM images of the local photocurrent generated at mono-bi layer graphene interfaces is performed to gain a more profound knowledge of the specific mechanisms governing electronic flow and resistivity at a nanoscopic level. In particular, by analyzing the polarity of the photocurrent concerning the source-drain voltage applied across the device, it was possible to indirectly image the charge carrier accumulation around a defect during electronic charge flow, predicted by Landauer in 1957. It was found that for values of the Fermi energies in proximity to the charge neutrality point (i.e. at low hole or electron doping) the photocurrent has the same polarity as the applied source-drain voltage, as it would be expected for changes in carrier concentration induced by the LRD.

HL 33.4 Wed 15:45 EW 201

**Energy- and Temperature-dependent Photoconductivity Studies for $MoSe_2$** — •Konstantin Neureither[1,2], Johannes Groebmeyer[1,2], Rao Peng[2], Johannes Knolle[2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut, TU Munich, Germany — [2]Physics Department, TU Munich

We study the photoconductivity of $MoSe_2$ for different excitations energies and lattice temperatures. Using circular polarized CW lasers, we focus on the effects of spin-orbit coupling on longitudinal and transversal photocurrents. Furthermore, we investigate a novel measurement technique that enables us to resolve long-time charge carrier decay dynamics by performing photocurrent spectroscopy in the frequency-domain.

HL 33.5 Wed 16:00 EW 201

**Persistent Photoconductivity in Thin Films of $ZrS_3$** — •Lars Thole[1], Asem Ben Kalefa[1], Christopher Belke[1], Sonja Locmelis[2], Lina Bockhorn[1], Peter Behrens[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

The field of two dimensional materials includes a large variety of materials. Among these, the group of transition metal trichalcogenides (TMTCs) has so far been lesser researched. Here, we have prepared transistor structures from thin films of the TMTC $ZrS_3$. In our samples, we found a particularly long persistent photoconductivity (PPC) which lasts over several hours, similar to what was seen in $MoS_2$ [2]. Looking at the temperature dependence gives information about the scattering times involved. In addition to using a stretched exponential function to fit the data, we can use a combination of three exponential functions. This shows that there are three processes involved in the origin of the PPC in our samples. These processes can be characterized by looking at samples with different thicknesses.

[1] L. Thole et al., ACS Appl. Electron. Mater., 5, 11, 6286 (2023)
[2] Y. Wu et al., Sci. Rep., 5, 11472 (2015)

# HL 34: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing II (joint session HL/DY/TT/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.

Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Wednesday 15:00–17:45 Location: EW 202

HL 34.1 Wed 15:00 EW 202

**Quantum backaction evasion in cavity magnomechanics** — •Victor Augusto Sant Anna V Bittencourt[1], Clinton A. Potts[2], John P. Davis[3], and Anja Metelmann[1,4,5] — [1]ISIS (UMR 7006), Universite de Strasbourg, 67000 Strasbourg, France — [2]Kavli Institute of NanoScience, Delft University of Technology, PO Box 5046, 2600 GA Delft, Netherlands — [3]Department of Physics, University of Alberta, Edmonton, Alberta T6G 2E9, Canada — [4]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76131, Karlsruhe, Germany — [5]Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

Magnetic excitations (magnons) hosted in a solid can couple to mechanical vibrations of the material (phonons) via a radiation-pressure like interaction due to magneto-elastic effects. When the magnet is loaded on a microwave cavity, phonons can be driven and measured via the microwave while having the tunability of the magnetic excitations. Nevertheless, the noise added to mechanics can hinders both potential applications of the system at the quantum level and measurements of the phonon mode. Here, we propose a scheme to evade quantum backaction on a phonon mode of a cavity magnomechanical system by using a two-tone microwave drive. We study the robustness of the different possible backaction evading schemes, and show that measurements of the phonon mode can be performed with added noise below the standard quantum limit.

HL 34.2 Wed 15:15 EW 202

**Optical detection of guided GHz acoustic phonons in a semiconductor hybrid microcavity** — •Mingyun Yuan[1], Antonio Crespo-Poveda[1], Alexander S. Kuznetsov[1], Klaus Biermann[1], Alexander Poshakinskiy[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5, 10117 Berlin, Germany — [2]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Spain

The interaction between acoustic phonons and optical quasiparticles has profound implication in both understanding of light-matter interaction and acousto-optical applications. We report on the optical detection of phonon echos resulting from the interaction between acoustic phonons and exciton polaritons in a hybrid (Al,Ga)As microcavity grown by molecular beam epitaxy. The microcavity spacer embedding multiple quantum wells is surrounded by Bragg mirrors designed to enable polariton formation. Simultaneously, the spacer-quantum wells and the Bragg reflectors act as the core and cladding regions, respectively, of an acoustic waveguide sustaining GHz acoustic phonons propagating along [110], excited by side bulk-acoustic-wave transducers. The acoustic modulation gives rise to an optical comb in the polariton photoluminescence, in which both the guided phonon modes and the substrate phonon modes are identified via Fourier transform. Our results demonstrate the robust generation of guided acoustic phonons above 6 GHz as well as their effective coupling to the polaritons, and showcase the sensitive optical detection of acoustic modes.

HL 34.3 Wed 15:30 EW 202

**Topological phononic waveguides with ultralow loss** — •Ilia Chernobrovkin[1], Xiang Xi[1], Jan Kosâta[2], Oded Zilberberg[3], Anders Sørensen[1], and Albert Schliesser[1] — [1]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark — [2]Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland — [3]Department of Physics, University of Konstanz, 78464 Konstanz, Germany

Topological insulators have long intrigued researchers in terms of fundamental physical properties as well as potential applications. The advantages of topological insulators have been extended to the realm of bosonic defects or waveguiding systems and overturned some of conventional views of photonic or phononic wave manipulation. However, the existing topological phononic waveguides still have large transportation loss, which limits its applications.

In our work, we combine the so-called soft-clamping technique - which can dramatically suppress mechanical losses - with non-trivial topology, designed to enable valley-locked propagation along a topological edge. Our systems are based on sub-100 nm thin, highly stressed membrane made of silicon nitride membranes. Our preliminary experimental results show a measured Q-factor above 1 million for whispering-galley megahertz-frequency elastic modes along a closed triangular path of length of ~10 mm, which corresponds to a classical coherent length of tens of meters. Our system can be considered promising for use in phononic circuits for coherent microwave signal processing or interconnection.

HL 34.4 Wed 15:45 EW 202

**Dry processing of high Q 3C-silicon carbide nanostring resonators** — •Felix David, Philipp Bredol, and Eva Weig — Technical University of Munich - Chair of Nano and Quantum Sensors, Garching, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. The conventional fabrication process involves electron-beam lithography with PMMA to define a metallic hard mask for the subsequent dry-etching step via a liftoff process. This requires some wet-chemical process steps, which can destroy our samples. Here we describe an alternative process, which avoids all wet-chemical process steps to enable superior quality. It involves the use of a negative electron-beam resist as an etch mask, as well as the completely reactive-ion etching-based release of the nanostrings. The dry-processed nanostrings can be fabricated with a high yield and exhibit high mechanical quality factors at room temperature. Due to the high reliability combined with the high process speed, it also allows us to investigate material-intensive questions, such as the influence of etching depth and undercut on the mechanical quality factor.

HL 34.5 Wed 16:00 EW 202

**Spatial Mode Mapping of 2D Mechanical Resonators** — •Lukas Schleicher, Leonard Geilen, Alexander Holleitner, and Eva Weig — TU München, Garching, Deutschland

We present studies on the spatial mapping of mechanical modes of 2D resonators based on monolayer transition-metal dichalcogenides. A spatially resolved mode mapping allows us to investigate non-isotropic pre-strain and other transfer-related artefacts, such as cracks and surface contaminations, which may result from the fabrication process. We compare the mechanical properties of drums with various sizes and fabrication methods of the 2D resonators.

**15 min. break**

HL 34.6 Wed 16:30 EW 202

**Electrochemical etching strategy for shaping monolithic 3D structures from 4H SiC wafers** — •André Hochreiter, Fabian Gross, Morris Niklas Möller, Michael Krieger, and Heiko Weber — Lehrstuhl für Angewandte Physik Universität Erlangen-Nürnberg, Germany

Silicon Carbide's (SiC) as wide bandgap semiconductor has outstanding material properties, which enable applications like already available commercial power-electric devices, and applications in quantum sensing. For mechanical applications of SiC, extremely high quality factors are predicted, but on-chip 3D shaping of SiC is difficult due to its chemical robustness. We report on an electrochemical etching (ECE) strategy, which solely relies on a doping contrast introduced by targeted ion-implantation of p-dopants on n-type material. With such a dopant-selective etching, n-doped regions remain inert and p-type regions are removed. We present devices as diverse as monolithic cantilevers, membranes and disk-shaped optical resonators etched out a single crystal wafer. The electrochemically etching process leaves the etched surface with low roughness, which can even be improved by annealing.

HL 34.7 Wed 16:45 EW 202

**Probing the Mechanical Loss of Individual Surfaces of a Nanomechanical String Resonator** — •Philipp Bredol, Felix David, and Eva Weig — Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

Stressed nanostring resonators are a promising platform for sensing applications and quantum technologies because of their small footprint and high mechanical quality factors. In this contribution we show that the dissipation caused by sidewall surfaces and the dissipation caused by bottom and top surfaces can be individually determined from the mechanical response spectrum. This information helps to evaluate and adjust fabrication parameters such as etchant chemistry, etch mask materials and possible annealing steps. Being able to characterize the mechanical loss mechanisms that limit a given device is important for integration with other structures and to further push the performance of nanostring resonators.

HL 34.8 Wed 17:00 EW 202

**Parametric normal mode splitting for coupling strength estimation** — •Ahmed A. Barakat, Avishek Chowdhury, Anh Tuan Le, and Eva M. Weig — Technical University of Munich, Munich, Germany

The experimental estimation of the linear coupling strength between two nanomechanical modes is a challenging task. For dielectrically actuated nano-string resonators, the coupling strength between in-plane and out-of-plane modes is usually estimated by tuning the modal eigenfrequencies using a bias voltage up to the occurrence of the avoided crossing. In this contribution, we introduce a novel approach using parametric excitation to estimate the linear coupling strength at any bias voltage.

In addition to a broadband noise excitation, the proposed approach involves parametrically driving in the direction of at least one of the eigenmodes with a frequency that resonates with the difference between both eigenfrequencies causing a parametric normal mode splitting. Using the dependence of the splitting width on the coupling strength, a mathematical model is introduced and perturbed around the parametric excitation frequency using the multiple scales method. The locus of the splitting is derived analytically and agrees well with the experimental results, leading to an accurate estimation of the coupling strength.

HL 34.9 Wed 17:15 EW 202

**Tunable near-infrared exciton-polariton optomechanical GHz rulers of light** — •Alexander Kuznetsov, Klaus Biermann, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Frequency combs, which consist of many equidistant optical lines, are photonic analogues of spatial rulers. Such rulers of light can be used for high-resolution spectroscopy, ranging, optical and atomic clocks, and for large-scale quantum systems. On-chip miniaturized and low-power comb-sources are, therefore, of great importance. Here, we demonstrate generation of tunable combs using spatially confined light-matter quasiparticles – exciton-polaritons – coherently modulated by GHz phonons inside a hybrid photon-phonon (Al,Ga)As patterned microcavity. Using non-resonant optical excitation, we create polariton Bose-Einstein-like condensates (BEC) with long temporal coherence reaching $\tau_{BEC} \approx 2$ ns. The BEC is modulated by piezoelectrically generated strain of bulk acoustic wave (BAW) phonons with frequency $f_{BAW} = 7$ GHz and RF-tunable amplitude. Since $\tau_{BEC} \gg 1/f_{BAW}$, the modulation is coherent and leads to the emergence of well-resolved phonon sidebands, separated by $f_{BAW}$, in the polariton emission spectrum. For large BAW amplitudes, the comb contains up to 50 well-resolved lines with nearly-flat profile. The demonstrated RF-induced comb functionality may be useful for the realization of on-chip arrays of tunable GHz optical combs as well as coherent optical-to-microwave bi-directional conversion.

HL 34.10 Wed 17:30 EW 202

**Imaging acoustic fields on metasurfaces** — •Alessandro Pitanti[1,2,3], Mingyun Yuan[1], Simone Zanotto[3], and Paulo Ventura Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 5-7 Hausvogteiplatz, Berlin 10117, Germany — [2]Dipartimento di Fisica E. Fermi, Università di Pisa, Largo B. Pontecorvo 3, Pisa 56127, Italy — [3]NEST, CNR Istituto Nanoscienze and Scuola Normale Superiore, piazza San Silvestro 12, Pisa 56127, Italy

The last decades have witnessed a rich activity towards the integration of acoustic technologies within electro-optical circuits in high-frequency hybrid devices. The main role in this trend has been played by surface acoustic waves (SAW), easily integrable in several material platforms via piezoelectricity. Given their high frequency and quality factors, simple SAW delay-line resonators have found application as sensors, filters, and oscillators for telecommunication applications. More complex manipulation of acoustic waves would boost SAW-based technologies, becoming a key for the transition to 6G; complete wave manipulation and control in the GHz range would offer the most promise for integration with modern communication technologies.

In this context, we illustrate the use of light-interferometry and atomic force microscopy based scanning probe techniques for a fine investigation of GHz acoustic fields in mechanical metasurfaces. Focusing on the role of symmetries in wave scattering, we show complex wave manipulation, leading to asymmetric negative refraction and anisotropic transmission of mechanical waves.

# HL 35: THz and MIR

Time: Wednesday 15:00–16:15 Location: EW 203

HL 35.1 Wed 15:00 EW 203

**Observation of picosecond Polaron Stabilization in FA-lead-halide pervoskites via infrared modes** — •Daniel Sandner[1], Matthias Nuber[1], Qi Ying Tan[2], Reinhard Kienberger[1], Cesare Soci[2], and Hristo Iglev[1] — [1]Chair for Laser- and X-ray physics E11, Technische Universität München, Garching, Germany — [2]Centre for Disruptive Photonic Technologies, NTU, Singapore

The optoelectronic properties of lead-halide perovskites are greatly influenced by the polarons. In our experiments, we use time-resolved mid-infrared spectroscopy with sub-ps and single wavenumber resolution to study the vibrational properties of the FA cation via a CN stretching mode. It has been shown in polymers and perovskites that localized charge carriers can lead to infrared active (IRAV) modes. After exciting Cs0.2FA0.8PbBr3 films with visible light pulses, we observe an IRAV mode that increases up to 100 ps after excitation in intensity, while the broad background by free carrier absorption shows a decline by carrier recombination. We interpret this finding as Polaron stabilization, meaning the rearrangement of the polar lattice around the charge carrier. (doi.org/10.1039/D2TC04519B)

We further studied the role of the halide, temperature, and confinement. At low temperatures, the IRAV mode, which we associate with a polaron, is weaker and shows shorter distinct dynamics, which is in good agreement with reported transport data. We find that the effect is absent in quasi-2D perovskites, which adds more experimental evidence to the recent debate about the nature of photoexcitations in those materials.

HL 35.2 Wed 15:15 EW 203

**Nonlinear terahertz responses of optically excited $Cu_2O$** — •Changqing Zhu, Anneke Reinold, Patrick Pilch, Marc Assmann, and Zhe Wang — TU Dortmund University, Germany

Excitons in $Cu_2O$ have attracted significant attention due to their peculiar properties, such as the remarkable Rydberg series with the principal quantum number extending up to 30 and the realization of Bose-Einstein condensation. We report on time-resolved nonlinear terahertz spectroscopic study of optically excited nonequilibrium states in $Cu_2O$. Terahertz harmonic generation is observed and investigated as a function of the fluence of the optical excitation and by varying the delay between the optical excitation and the terahertz driving pulse. Our time-resolved spectroscopic techniques allow us to associate the observed nonlinear terahertz responses with different processes of exciton-related dynamics.

HL 35.3 Wed 15:30 EW 203

**Mid-infrared photocurrents in topological insulator thin film** — •Filippo Romano[1,2], Holger Mirkes[1,2], Nina Pettinger[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institute and Physik-Department, Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Clearly discriminating the transport of trivial bulk and non-trivial surface states remains often challenging in topological insulators because of their rather large residual bulk conductivity. Photogalvanic currents can serve as a tool to selectively address the surface states based on simple symmetry principles (Nanophotonics 2020, 9, 2693 - 2708). However, most experiments so far used a near-infrared excitation far above the fundamental bulk gap of the prototypical 3D topological insulators mixing surface and bulk states in the optical excitation process (Nat. Commun. 2015, 6, 6617). Here, we extend optoelectronic measurements of topological insulator thin films from near-infrared (from 0.8 $\mu$m) to mid-infrared wavelengths (up to 20 $\mu$m). The latter may allow a selective excitation of surface state photocurrents without contribution from bulk bands. The research is supported through the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No 101076915 (2DTopS).

HL 35.4 Wed 15:45 EW 203

**Cyclotron and spin resonances in AlAs quantum wells** — •Daniiar Khudaiberdiev — Institute of Solid State Physics, Vienna University of Technology, Vienna, 1040, Austria

Magneto-optical spectroscopy in THz range is a very useful technique for studying two-dimensional electron systems (2DESs). The main effect that is usually measured is the cyclotron resonance (CR), which gives the information on the cyclotron mass of the charged carriers, and thus, can be used to reconstruct the band structure in some cases [1]. Recently, a different method of measuring the effective mass was introduced [2]. This interferometric method gives the conductivity mass that, in contrast to the cyclotron mass, can be renormalized by the electron-electron interaction and also can be anisotropic. In this work we are using both methods to probe the AlAs quantum well system, which is well known for it*s anisotropic and heavy effective mass, and therefore, for it*s strong electron-electron interaction [3]. *In addition to the cyclotron resonance, the electron spin resonance (ESR) have also been observed in the system. Both of them are present in both photoresistance and transmission data. Direct observation of the ESR in the optical response provides an opportunity to study its polarization dependencies, that can give new information on its nature. [1] J. Gospodarič et al., Phys. Rev. B 104, 115307 (2021). [2] V. M. Muravev et al., Phys. Rev. Applied 19, 024039 (2023) [3] A. V. Shchepetilnikov et al., Phys. Rev. B 92, 161301(R) (2015).

HL 35.5 Wed 16:00 EW 203

**Simulation and measurement of silicon resistivity characterization with terahertz TDS** — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Christian Röder[3], Kuei-Shen Hsu[4], Jan Beyer[4], Nadine Schüler[5], 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]Fraunhofer Institute for Integrated Systems and Device Technology IISB, Department Energy Materials and Test Devices, Erlangen — [4]Institute of Applied Physics, Technische Universität Bergakademie Freiberg — [5]Freiberg Instruments GmbH, Freiberg

Silicon is one of the most important semiconductors used in many applications that are essential to modern electronics. One of its main characteristics is the resistivity which is usually measured by the four-point probe method requiring to contact the sample with the measuring tip. This, however, always contains the danger of affecting the material under test. A fast and non-contact measurement technique is terahertz time-domain spectroscopy (TDS). This technique is already well established in the characterization of dielectrics, but its potential to characterize semiconductors is not fully utilized, yet. Therefore, this potential is investigated by simulations as well as measurements of single-layer silicon wafers as well as two-layer silicon samples with TDS. As will be shown, the resistivity characterization is possible over a wide range for single-layer samples, while it is more complicated and restricted to specific cases for two-layer samples.

# HL 36: Poster III

Topics:
- 2D semiconductors and van der Waals heterostructures
- Functional semiconductors for renewable energy solutions
- Nanomechanical systems for classical and quantum sensing
- Nitrides

Time: Wednesday 18:00–20:30 Location: Poster E

HL 36.1 Wed 18:00 Poster E

**Entangled two-photon absorption in 2D semiconductors** — •Till Weickhardt and Giancarlo Soavi — Institute of Solid State Physics, Jena, Germany

The excitonic states in TMDCs lead to resonant enhancement of SHG and two-photon absorption (TPA) with huge cross-sections and have been proposed as gates for valleytronics.[1] To generate detectable populations of excitons in two photon processes with classical light and not damaging the monolayer it is necessary to use a pulsed laser with a broad spectrum. This limits the energy resolution of any experiment. In this work, we propose a possible way to remedy this problem by using energy-time entangled photons from spontaneous parametric down conversion (SPDC). This way, the photons are temporally synchronized in pairs and sum up to a precise and narrow energy spectrum while the distribution of single-photon energies can be broad.[2] This leads to higher efficiencies for TPA combined with spectral resolution beyond the Fourier limit. Entangled two-photon absorption (ETPA) has been demonstrated in fluorophores but never in solid-state systems.[3] To achieve this, two experimental requirements must be met: (i) a tunable narrowband laser to precisely hit the excitonic resonances of the TMDC under investigation. (ii) a SPDC source with high photon-pair flux, leading to an average power of at least 100 nW. While these requirements have already been met in our labs, first measurements of ETPA in TMDCs are still pending at this stage.

References: [1]Herrmann et al., Small 19, 2301126(2023) [2]Dayan et al., PRL 94, 043602(2015) [3]Tabakaev et al., PRA 103, 033701(2021)

HL 36.2 Wed 18:00 Poster E

**Photoluminescence of Organic-Dye/TMD Hybrid Structures** — •Julian Schröer, Lisa Böhme, Erik von der Oelsnitz, Alina Schubert, Rico Schwartz, Stefan Lochbrunner, and Tobias Korn — University of Rostock, Institute of Physics, AG Zweidimensionale Kristalle und Heterostrukturen

Thin layers of organic molecules and layered semiconductors build a new compound material with many interesting applications. The optoelectronic properties of these heterostructures strongly depend on the chosen compounds. In our work, we apply photoluminescence spectroscopy to hybrid structures of the organic dye perylene orange (PO) combined with monolayers of transition metal dichalcogenides (TMDs) like MoSe2, MoS2 and WSe2. These hybrid structures are candidates for fast and efficient charge or energy transfer due to their emerging type-II band alignment. Here, we aim to reveal the charge transfer processes in the different heterostructures by examining the excitation density-dependent low-temperature photoluminescence of the exciton and trion of the TMDs. Our work paves the way for a deeper understanding of organic/inorganic heterointerfaces and their application as photodetectors or light-harvesting devices.

HL 36.3 Wed 18:00 Poster E

**Time-resolved Faraday ellipticity on multilayer $WSe_2$** — •Anna Weindl[1], Jennifer Lehner[1], Simon Raiber[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 mulitlayers of the transition metal dichalcogenid $WSe_2$. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the temporal dynamics in $WSe_2$ multilayers. These previous results have shown that pseudospin oscillations appear in the TRFE signal when we apply an in-plane magnetic field to our samples. Now we try to characterize and manipulate these oscillations by playing with different experiment 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] S. Raiber, P. E. Faria Junior, D. Falter, S. Feldl, P. Marzena, K. Watanabe, T. Taniguchi, J. Fabian, C. Schüller. Ultrafast pseudospin quantum beats in multilayer $WSe_2$ and $MoSe_2$, Nat. Commun. 13, 4997 (2022).

HL 36.4 Wed 18:00 Poster E

**Giant band Splitting in WSe2/WTe2 heterostructure** — •jiabao yang[1], wei yao[1], pavel dudin[2], jose avila[2], stuart parkin[1], and niels schröter[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg2, 06120 Halle(Saale), Germany — [2]Synchrotron SOLEIL, L*Orme des Merisiers , Saint Aubin BP 48, 91192 Gif sur Yvette Cedex, France

Two-dimensional (2D) heterostructures have emerged as a promising platform for investigating strongly correlated electronic phases. Transport measurements on WSe2/WTe2 have shown a switchable correlated insulating state by a ferroelectric field, but clearer evidence on how interlayer interaction and the formation of the Hubbard bands are influenced by ferroelectricity is still lacking. Based on Angle-Resolved Photoemission Spectroscopy (ARPES), we have found two interesting phenomena, the giant band splitting in the WSe2 layer with a ferroelectric WTe2 substrate, and the splitting of the bilayer WTe2 conduction band under the Moiré potential by WSe2.

HL 36.5 Wed 18:00 Poster E

**Enhanced light-matter interaction in a monolayer of WS2 on top of Mie voids in a high-index material** — •Padam Nagarkoti[1], Serkan Aslan[2], Hossein Ostovar[1], Mario Hentschel[2], Harald Giessen[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany

Light manipulation in subwavelength structures has gained significant attention in recent years. It is mostly based on the optical resonances in the metallic and dielectric materials. In this work, we numerically study the optical properties of Mie voids[1] created in the high index material using finite element method simulation. We calculate and visualize the electric field within the system, illuminating Mie voids from above. The simulation result shows that the light is entirely localized and confined within the void. Peaks in the reflectance spectra indicate resonant modes. We demonstrate that the resonance wavelength can be shifted by changing the dimensions of the void. Increasing either the height or diameter or both dimensions of the void, a red shift in the resonance wavelength is found. Furthermore, we show the coupling of resonant modes with WS2 monolayer on top of the void results in enhanced absorption. The absorption in the WS2 is optimized by tuning the void parameters. These results indicate that the 2D semiconducting materials in combination with Mie voids have a great potential for light trapping and solar energy conversion applications.[1] Hentschel et al. Light: Science & Applications (2023) 12:3

HL 36.6 Wed 18:00 Poster E

**Optoelectronic Control of Interlayer Excitons in $MoSe_2/WSe_2$ Heterostructures** — •Jan-Niklas Heidkamp[1], Johannes Krause[1], Swarup Deb[1], Takashi Taniguchi[2], Kenji Watanabe[2], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]National Institute for Material Science, Tsukuba, Japan

Transition-metal dichalcogenide (TMDC) heterostructures have recently garnered significant scientific interest due to their unique optical properties, including the emergence of tightly bound intralayer excitons and long-lived interlayer excitons. In this study, we investi-

gate the photoluminescence (PL) associated with interlayer excitons in heterostructures comprising molybdenum diselenide ($MoSe_2$) and tungsten diselenide ($WSe_2$). We aim to manipulate these quasiparticles using in-plane electric fields and modulation of the charge carrier density applied via microstructured electrodes and a potential difference across the heterostack. These experimental investigations provide valuable insights into the optical properties and behavior of interlayer excitons in TMDC heterostructures, offering prospects for their potential application in optoelectronic devices and photonics.

HL 36.7 Wed 18:00 Poster E

**Amplification of interlayer exciton emission in twisted WSe2/WSe2/MoSe2 heterotrilayers** — •Chirag Palekar[1], Paulo E. Faria Junior[2], Bárbara Rosa[1], Frederico Sousa[3], Leandro Malard[3], Jaroslav Fabian[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais 30123-970

Transition metal dichalcogenides (TMDC) heterostructures (HS) obtained by stacking two or more different monolayers (ML) host interlayer excitons (IX) with unique properties that depend on the twist angle and stacking order of MLs. However, IX*s practical applications are limited by the weak oscillator strength, leading a significant reduction in emission. Hence a viable path towards substantially improving the emission of IX is desirable. Here we investigate the twist angle dependent enhancement of IX emission in WSe2/WSe2/MoSe2 heterotrilayer (HTL) systems. The IX exciton formed in the HTL region exhibits a up to 10-fold increase in PL yield compared to HBL region on the same sample [1]. To understand the enhancement of the IX emission, we performed DFT calculations and effective modelling of the low energy IX states. This fundamental study of excitons in HTL system deepens the current understanding of twisted TMDC HSs and paves the way for further experiments, theoretical work and applications. [1] Palekar et al. arXiv:2311.02509,2023

HL 36.8 Wed 18:00 Poster E

**Machine Learning based Monolayer Classification using a Convolutional Neural Network and Characterization of Transition Metal Dichalcogenides Heterostructures** — •Maximilian Nagel, Chirag Palekar, Bárbara Rosa, Ching-Wen Shih, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

This research presents an advancement in the mass production of transition metal dichalcogenides (TMDCs) with potential benefits for the semiconductor industry. We introduce an automated system using convolutional neural networks (CNNs) for identification, classification and streamlining the monolayer search. Additionally, our study utilizes photoluminescence and second harmonic generation measurements for precise twist angle determination of heterostructures which are prepared using dry transfer method. By integrating data acquisition, image analysis, and machine learning, this innovative approach aids the TMDC heterostructure fabrication and enhances our understanding of TMDC heterostructures' properties. Collectively, this work represents a significant step forward in achieving cost-effective and efficient thin film manufacturing, with substantial implications for the semiconductor industry's future competitiveness and innovation.

HL 36.9 Wed 18:00 Poster E

**Properties and Defects of hexagonal boron nitride grown by pulsed laser deposition** — •Daniel Klenkert[1,2], Benedikt Winter[1], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University of Würzburg, 97074 Würzburg

Hexagonal boron nitride (hBN) has recently attracted significant research interest due to its unique properties. These include the chemical stability, its wide bandgap and the ability to host color centers inside the bandgap. These color centers exhibit bright and stable single photon emission at room temperature, which makes them interesting candidates for applications such as quantum communication and quantum sensing. To enable the direct pumping of color centers we examine the possibility to deposit hBN directly on LED and laser diode facets. As an intermediate step in this development, we report the results from spectroscopic measurements of hBN layers grown by pulsed laser deposition on silicon substrates as well as first tests on LEDs.

HL 36.10 Wed 18:00 Poster E

**Enhanced room-temperature spin-valley coupling in Vanadium-doped MoS2** — •Krishna Rani Sahoo[1,2], Janmey Jay Panda[1], Sumit Bawari[1], Rahul Sharma[1], Dipak Maity[1], Ashique Lal[1], Raul Arenal[3], G Rajalaksmi[1], and Tharangattu N. Narayanan[1] — [1]Tata Institute of Fundamental Research-Hyderabad, Sy. No. 36/P, Gopanapally Village, Serilingampally Mandal, Hyderabad-500046, India — [2]Institute of Physics, University of Münster, Wilhelm-Klemm-Straße 10 48149 Münster, Germany — [3]Fundación ARAID, 50018 Zaragoza, Spain

Achieving room-temperature valley polarization in atomically thin materials by substitutional doping opens new avenues of spintronic applications. Here, we demonstrate that monolayer MoS2 (MS) doped with vanadium (V) at low concentrations exhibits high spin-valley coupling and hence a high degree of valley polarization at room temperature. A time-reversal symmetry broken energy shift in the equivalent valleys is predicted in V-doped MoS2 (VMS). Our room-temperature chirality-controlled photoluminescence excitation measurements indicate such a shift in valley exciton energies (~35 meV). An enhanced valley polarization in VMS (~42%) is observed in comparison to that in MS (<12%), while in MS, the chirality-controlled excitations did not show a difference in emission energies. Spin Hall effect of light-based optical rotation measurements indicate the asymmetric absorption among the two different chiralities of the incident light, hence supporting the existence of room-temperature valley polarization.

HL 36.11 Wed 18:00 Poster E

**Optical characterization of non-magnetic 2D semiconductor MgPS3 and magnetic 2D semiconductor MnPS3** — •Thomas Kliewer[1], Pierre-Maurice Piel[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

The van-der-Waals (vdW) materials MnPS3 and MgPS3 are members of the metal phosphorus trichalgonides family (MPX3) which has recently gained interest due to its wide range of physical and chemical properties. MgPS3 is a possible photocatalyst for water-splitting reactions [1]. MnPS3 exhibits a ferromagnetic configuration between adjacent layers and an antiferromagnetic order in the layers [2] making it interesting for fundamental studies on magnetism in the 2D-limit.

Here we report on photoluminescence (PL)- and non-resonant Raman-spectroscopy investigations to characterize the optical and vibrational properties of both materials. To probe the impact of magnetic ordering, MnPS3 has been studied as function of temperature across the Néel-temperature.

For below-band gag excitation we find emission signatures in MnPS3 suggesting the existence of optically active in-gap states most likely due to defects. The Raman spectra of MnPS3 show the expected Raman active phonon modes. For MgPS3 the Raman-spectra show large intensity variations between different samples with different thickness.

[1] Jan Paštika et al. Small 18.18 (2022), p. 2200355 [2] Ko Kurosawa et al. J. Phys. Soc. Jpn. 52 (1983), pp. 3919-3926

HL 36.12 Wed 18:00 Poster E

**Moiré Minibands, twist disorder and exciton-phonon coupling in van der Waals stacks** — •Hendrik Lambers[1], Nihit Saigal[1], Nicolai-Leonic Bathen[1], Veljko Antic[1], Lennart Klebl[2], Dante M. Kennes[3], Tim O. Wehling[2], and Ursula Wurstbauer[1] — [1]University of Münster, Münster, Germany — [2]University of Hamburg, Hamburg, Germany — [3]RWTH Aachen University, Aachen, Germany

The weak van der Waals coupling between layers of most two-dimensional (2D) materials allows the realization of precisely tailored 2D quantum systems. Twisted homobilayers such as $tWSe_2$ are prone to the formation of moiré minibands. Guided by theoretical prediction, we study $tWSe_2$ homobilayer encapsulated in hBN by low-temperature resonant inelastic light scattering (RILS). We find resonant modes interpreted as single-particle collective inter-moiré-band excitations (IMBE) allowing to quantitatively probe the formation of a series of moiré-bands [1]. Moreover, we find that the resonance profiles particularly of the degenerated $WSe_2$ $A_1$'/E' phonon modes are significantly impacted by the assembly in vdW stacks suggesting a higher order Raman scattering process presumably involving simultaneous excitation and annihilation of phonon modes with finite momentum. [1] N. Saigal et al., arXiv:2310.14417 (2023).

HL 36.13 Wed 18:00 Poster E

**Gas sensing of $WSi_2N_4$ in dark and bright environments** — •Mustapha Driouech, Muhammad Sufyan Ramzan, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Two-dimensional materials are highly promising for gas sensing. In this work, we investigate the adsorption of the three common environmental gas molecules, namely $O_2$, $CO_2$, and $H_2O$ on monolayer $WSi_2N_4$. Using density functional theory, we simulate molecular adsorption and evaluate resulting changes in the electronic structure of the monolayer in the dark and bright environment. The latter (former) is mimicked by promoting (removing) an electron to the conduction (valance) state. Our results show that all gas molecules are physically adsorbed on the $WSi_2N_4$ surface with small charge transfer in the dark. The presence of photogenerated electrons and holes changes the strength of gas adsorption. While with $CO_2$ and $H_2O$ $WSi_2N_4$ behaves similarly in the dark and light environment, bright conditions enhance the interaction of $WSi_2N_4$ with $O_2$. As a result, charge transfer is increased compared to the dark, and substrate oxidation is promoted. Moreover, in terms of electronic properties, $O_2$ molecules contribute to the valence band maximum of the system regardless of the environment, making $WSi_2N_4$ a promising material for oxygen sensing.

HL 36.14 Wed 18:00 Poster E

**Theory of Phonon Sidebands in the Absorption Spectra of Moiré Exciton-Polaritons** — •Kevin Jürgens[1], Daniel Wigger[2], and Tilmann Kuhn[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany

Excitons in twisted bilayers of transition metal dichalcogenides experience a spatially varying electronic environment, which manifests in the formation of a periodic and twist-angle dependent moiré potential. For small twist angles the excitons are localized at the minima of the moiré potential, resulting in a flat band structure, whereas for large twist angles the excitons are almost entirely delocalized. When placing the heterostructure in an optical cavity, the moiré excitons interact with the photonic field, which leads to the formation of moiré exciton-polaritons. These couple to the lattice vibrations of the heterostructure giving rise to transitions between the two polariton branches that strongly depend on the twist angle.

We calculate the absorption spectra in the limit of small polariton densities. The polaritons are coupled to the same phonon bath, which results in inter- and intrabranch transitions in the polariton dispersion. We analyze the spectra and find rich phonon sidebands reflecting optical transitions assisted by phonon emission or absorption, that strongly depend on the twist angle. We identify the polariton gap and the presence of Van Hove singularities as critical parameters.

HL 36.15 Wed 18:00 Poster E

**Investigating the Electrical Performance of Exfoliated Mono-Layer and Few-Layer Graphene** — •Yasaman Jarrahi Zadeh, Felix Schaumburg, Jens Kerski, Günther Prinz, Martin Paul Geller, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

The groundbreaking discovery of two-dimensional (2D) graphene in 2004 sparked immense interest owing to its extraordinary electrical properties. Graphene's exceptional electron mobility makes it an ideal material for semiconductor devices that require fast response times. Additionally, the number of layers of graphene affects its different properties [1]. This study investigates the electrical behavior of exfoliated mono-layer and few-layer graphene structures on a Si substrate with SiO_2 top layer. To accomplish this, we employ the Van der Pauw method and Hall effect measurements to comprehend conductivity, carrier mobility, and quantum transport phenomena in both mono-layer and few-layer graphene. However, the characterization of ultrathin 2D material-based devices using electrical techniques poses challenges, and the conventional methods of characterization require optimization. By obtaining the electrical properties of graphene most optimally, further steps will be to enhance the performance of semiconductor devices like transistors and photodetectors.

[1] Urade, A.R., Lahiri, I. & Suresh, K.S. Graphene Properties, Synthesis and Applications: A Review. JOM 75, 614-630 (2023).

HL 36.16 Wed 18:00 Poster E

**Nonlinear optical observation of time-reversal symmetry breaking in graphene** — •Nele Tornow, Omid Ghaebi, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany

Monolayer graphene (MLG) provides the ideal platform to study the interplay between space inversion symmetry (IS), time-reversal symmetry (TRS), and topology [1]. The development of new ultrafast and non-perturbative all-optical spectroscopy methods could provide invaluable insights in this context, and nonlinear optics (NLO) is a promising approach thanks to its sensitivity to crystal symmetries.

In this work, we use NLO spectroscopy to investigate breaking of TRS in MLG, while preserving IS. To this end, we excite a MLG field-effect transistor with elliptically polarized light, i.e. with perfectly time and space superimposed and degenerate circular (pump) and linear (probe) beams. The circular pump breaks TRS, while the linear component probes the new terms generated in the NLO susceptibility, which result in a rotation of the emitted third-harmonic (TH) signal, in analogy with the valley nonlinear Kerr rotation observed in transition metal dichalcogenides [2]. Preliminary results further show a rotation of the TH signal as a function of both doping and excitation power.

Our results demonstrate a new method for all-optical generation and detection of broken TRS in MLG and thus a new powerful tool to explore topology in centro-symmetric crystals.

[1] McIver, J. W. et al., Nat. Phys. 16, 38-41 (2020)
[2] Herrmann, P. et al., Small 19, e2301126 (2023)

HL 36.17 Wed 18:00 Poster E

**Optically gated acousto-electric effect in 2D semiconductors** — •Felix Ehring, Benjamin Mayer, Clemens Strobl, Matthias Weiss, 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 nanosystems. In our experiments we fabricated hybrid lithium niobate SAW-devices including SAW delay lines with design frequencies of 150-250MHz containing gold electrodes on which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials can be placed. The dynamic electric field of the SAW induces a SAW power-dependent Acousto-Electric Current (AEC) in the different TMDC structures. The SAW directional dependence of this fundamental effect enables a detailed investigation of the TMDC interface.Through the spatially-resolved photodoping of the TMDC with a focused green laser (532nm), this setup can be utilized to study the charge carrier dynamics in a variety of different TMDCs, spanning from mono- to few-layer. [1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 36.18 Wed 18:00 Poster E

**Pump-probe spectroscopy of Rydberg excitons in TMDC monolayers** — •Max Wegerhoff, Moritz Scharfstädt, Andrea Bergschneider, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Quantum photonic technologies rely on strong optical nonlinearities, such as those provided by Rydberg atoms. The solid-state analog to this are Rydberg excitons. Rydberg excitons in cuprous oxides with principal quantum numbers of up to n=25 show strong optical nonlinearities, whose signatures could be detected by pump-probe spectroscopy [1]. In TMDC monolayers, which exhibit particularly strongly bound excitons, an increased nonlinearity could already be established for exciton-polaritons with n=2 [2].

Here, we report on the pump-probe spectroscopy of Rydberg states of excitons in TMDC monolayers at liquid helium temperatures. We use spectrally broad femtosecond probe pulses and a spectrometer to measure the transient differential reflectivity spectra. The degenerate pump-pulses are suppressed in a cross-polarized configuration such that the same Rydberg state is excited and probed. The doping of the monolayers is defined by electrical gating and kept neutral for the measurements.

[1] Heckötter, J., Walther, V., Scheel, S. et al., Nat Commun 12, 3556 (2021)
[2] Gu, J., Walther, V., Waldecker, L. et al., Nat Commun 12, 2269 (2021)

HL 36.19 Wed 18:00 Poster E

**Photoluminescence emission of TMDC Monolayers under strain** — •Pabin Rai, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Wilhelm-klemm-straße 10 48149 Münster Ger-

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Monolayers of transition metal dichalcogenides (TMDC) emit considerable photoluminescence despite their atomic thickness. The band gap of monolayers decreases when subjected to unidirectional mechanical tensile strain, resulting in a redshift in photoluminescence. Typically, uniaxial tensile strain is applied by bending a flexible polymer with a TMDC monolayer on top. However, this method causes strong sample displacement in the focusing direction, requires realignment after every strain step, and prevents the usage of high-numerical-aperture objective lenses. Here we demonstrate strain application by linearly pulling the flexible polymer substrate to circumvent these issues. These findings bear significance in advancing the development of strain-tuned optoelectronic devices.

HL 36.20 Wed 18:00 Poster E

**Electrical transport properties of twisted bilayer graphene with twist angle disorder** — •Bei Zheng, Xiaoyue Zhang, Fan Bai, Lina Bockhorn, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The twisting of the graphene layer opens up a whole new field of rich physics [1]. Especially, the electronic properties of twisted bilayer graphene depend strongly on the twist angle[2,3]. The twisted graphene structures around the magic angle were the first systems to show strong correlation behaviors, such as the rise of superconductivity and Mott's insulating phase [4,5].

We fabricated two twisted bilayer graphene samples around the magic angle via the "tear and stack" method. We investigated their transport properties by carrying out field effect measurements at different temperatures $T$ from 300 K down to 1.4 K. The samples showed signatures of twist angle disorder and the resulting quantum interference. We analyzed the temperature- and carrier density-dependent conductance fluctuation $\Delta G_{xx}$ and concluded that, although the disorder of twist angle suppresses the superlattice effect and enhances the quantum interference, the coexistence of phase transition and quantum interference still can be observed since the phase-coherence length $L_\phi$ is one order of magnitude larger than the moiré superlattice constant $\lambda_m$ for both samples. [1] H. Schmidt et al., Nat. Commun. 5, 5742 (2014) [2] J. C. Rode et al., 2D Mater. 3, 035005 (2016) [3] S. J. Hong et al., 2D Mater. 8, 045008 (2021) [4] Y. Cao et al., Nat. 556, 43-50 (2018) [5] X. Lu et al., Nat. 574, 653-657 (2019)

HL 36.21 Wed 18:00 Poster E

**Anisotropic transport in 1D Bilayer Graphene Superlattices** — •Julia Amann[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

One-dimensional superlattices (1DSLs) in graphene have been predicted to show intriguing effects, such as transport anisotropy, additional Dirac points and a distorted Fermi contour. In contrast to two-dimensional graphene superlattices, which have been widely studied, only very few experiments on 1DSLs have been reported. We use a patterned few-layer graphene gate underneath an encapsulated bilayer graphene to create a 1DSL. With the combined action of a global gate and a patterned bottom gate we can control superlattice potential strength and charge carrier density independently. We show low temperature transport measurements on a gate tunable 1DSL in bilayer graphene with a period of 50 nm in directions parallel and perpendicular to the modulation as we use a L-shaped Hallbar. We observe anisotropic transport in x and y directions and the appearance of multiple Dirac points in the modulation direction. These extra Dirac points are represented as additional Landau fans in magnetotransport. Furthermore, Weiss-oscillations are observed confirming the 1DSL modulation and the anisotropy.

HL 36.22 Wed 18:00 Poster E

**Substitutional Doping of Exfoliated 2D Materials** — •Sirri Batuhan Kalkan[1], Felix Junge[2], Hans Hofsäss[2], and Thomas Weitz[1] — [1]I. Institute of Physics, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]II. Institute of Physics, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Low-energy (<50 eV) ion implantation is a versatile technique for creating novel two-dimensional electronic devices by doping with electrons, holes, or inducing magnetism [1-3]. These modified films can be utilized as electrodes in energy-efficient electrochemical processes, homojunctions of the same material, or unique spintronic devices. In this poster, we discuss the optimization of the implantation processes for mechanically exfoliated 2D materials. We cover several topics, including improvements through post-cleaning approaches, the influence of doping-induced defects, the fabrication of prototype van der Waals heterostructure devices, and their characterization.

References: [1] Willke, Philip, et al. "Doping of graphene by low-energy ion beam implantation: structural, electronic, and transport properties." Nano Letters 15.8 (2015): 5110-5115 [2] Lin, Pin-Cheng, et al. "Doping graphene with substitutional Mn." ACS nano 15.3 (2021): 5449-5458. [3] Pramanik, Arindam, et al. "Anomalies at the Dirac Point in Graphene and Its Hole-Doped Compositions." Physical Review Letters 128.16 (2022): 166401

HL 36.23 Wed 18:00 Poster E

**Wavelength-Dependent Optical Excitation and Depth-Resolved Photoluminescence Spectroscopy of Defects in hexagonal Boron Nitride** — •Diana Gühring[1], Paul Konrad[1], Lina M. Todenhagen[2], Andreas Sperlich[1], Igor Aharonovich[3], Martin S. Brandt[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [2]Walter Schottky Institute and School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

In recent years, quantum emitters in 2D materials, such as hexagonal Boron Nitride (hBN), have shown promising applications in various fields of quantum technology. Although the recently discovered boron vacancy ($V_B{}^-$) spin-defect center in hBN is especially promising for nanoscale sensing, a deeper insight into its optical properties remains unexplored. Here, the wavelength-dependent optical excitation in correlation with photoluminescence (PL) is investigated to gain insights into the fundamental characteristics of $V_B{}^-$. Furthermore, the study includes confocally resolved, depth-dependent PL spectroscopy, examining the impact of the environment on the observed PL. The findings presented here contribute to a comprehensive understanding of the optical properties of defects in hBN, offering valuable insights for an efficient exploitation of this promising quantum material.

HL 36.24 Wed 18:00 Poster E

**Towards magnetotransport measurements in rhombohedral penta-layer graphene** — •David Urbaniak, Christian Eckel, Anna Seiler, and Thomas Weitz — University of Göttingen, Faculty of Physics, 1st Institute of Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Graphene is one of the most studied 2D material to-date. Due to its band structure, rhombohedrally stacked multi-layer graphene has been the subject of recent studies. Notably the discovery of superconductivity in tri-layer graphene attracted significant attention [1]. Penta-layer graphene is currently of particular interest for the study of electron correlation effects due to its high density of state stemming from increased flat bands near the band edge [2, 3]. This work shows how rhombohedrally stacked regions of mechanically exfoliated penta-layer graphene can be identified via Raman spectroscopy and spatially resolved in the nanometer regime by scanning near field optical microscopy (SNOM). Furthermore, a nanolithography technique to isolate such regions using an atomic force microscope (AFM) is presented, as well as the fabrication steps of hexagonal Boron Nitride (hBN) encapsulated dual gated magnetotransport devices and the stability of the rhombohedral stacking order during the fabrication process. Additionally, an outlook on the upcoming magnetotransport measurements in the milli Kelvin regime is discussed.

References: [1] Zhou, Haoxin, et al. Nature 598.7881 (2021): 434-438. [2] Han, Tonghang, et al. Nature 623, 41-47 (2023) [3] Han, Tonghang. et al. Nat. Nanotechnol. (2023)

HL 36.25 Wed 18:00 Poster E

**Multi-method characterization of initial growth of a $MoS_2$ layer by atomic layer deposition** — •Christian Petersen, Christian Tessarek, Alexander Karg, Alexander Hinz, Niels Osterloh, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

$MoS_2$ is a 2D semiconductor with exceptional optical and electrical properties, thus considered as a possible future material for ultra-thin film transistors or optoelectronic devices. To overcome size limitations due to exfoliation, synthesis methods like chemical vapour deposition or atomic layer deposition (ALD) bear the possibility for large scale controlled fabrication of pristine monolayers.

In this comprehensive study $MoS_2$ layers grown by ALD from submonolayer to the bilayer regime are analyzed. The surface morphology was investigated by atomic force microscopy (AFM). In addition, X-ray photoelectron spectroscopy (XPS) was used for a chemical analysis while Raman as well as photoluminescence (PL) spectroscopy revealed structural and optical properties. In combination of these methods the monolayer growth regime was identified and a growth model is proposed that is used explain the obtained results.

HL 36.26 Wed 18:00 Poster E

**Resonant and non-Resonant Raman spectroscopy on the magnetic semiconductor CrSBr** — •Oskar Schröer[1], Pierre-Maurice Piel[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

CrSBr, a van der Waals (vdW) material, exhibits a remarkable combination of attributes. It is an optically active, air-stable magnetic semiconductor, and its vdW structure endows it with magnetic properties characterized by ferromagnetic ordering within each layer and antiferromagnetic coupling between adjacent layers. This unique electronic band structure imparts strong anisotropy, effectively transforming the material into a quasi-one-dimensional system [1]. As a result, CrSBr's direct band gap is marked by robust, anisotropic excitonic resonances, rendering it particularly intriguing to study interaction physics. For opto-spintronic applications, it is imperative to cultivate a profound understanding of its quasi-particles, their interactions, and their intricate interplay with magnetic order. Here, we report on temperature dependent photoluminescence (PL) as well as resonant and non-resonant Raman spectroscopy experiments below and above the Néel temperature to study the impact of the magnetic ordering in bulk CrSBr. We find that peculiar signatures only observable in resonant Raman spectra are indicative for the magnetic phase transition from the anti-ferromagnetic to the paramagnetic state. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023)

HL 36.27 Wed 18:00 Poster E

**Interlayer excitons engineering in Transition Metal Dichalcogenides Heterobilayer** — •Ridha Eddhib, Aki Pulkkinen, and Jan Minar — New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic.

Our study is aimed to showcase the feasibility of manipulating the optical characteristics of transition metal dichalcogenide Heterostructures (TMD-HS) beyond the intralayer excitons[1-2], particularly when one of the constituent layers adopts a ternary structure which is an intriguing class of HS known as type II band alignment. This manipulation bears crucial implications for enhancing charge separation efficiency, as optically excited electrons and holes undergo relaxation into distinct material layers giving rise to interlayer excitons. In the realm of binary-ternary (B-T) HS systems, we have investigated the exciting avenue for extending the energy range and tailoring emission energies, surpassing the capabilities of their (B-B) and free standing counterparts. Our findings underscore the significance of the alloying ratio in fine-tuning excitons binding energy, and also highlighting the importance in the band offset in the emergence of this optical feature thereby introducing a novel design parameter for tailoring optoelectronic devices to specific applications. [1] Hichri, A., T. Amand, and S. Jaziri. Physical Review Materials 5.11 (2021): 114002. [2]Aly, M. A., Enakerakpor, E. O., Koch, M., & Masenda, H. (2023). Nanomaterials, 13(20), 2769.

HL 36.28 Wed 18:00 Poster E

**Ion-irradiated hBN-silicon hybrid photodetectors for near infrared polarized imaging** — •Peiting Wen[1,2], Mohd Saif Shaikh[1,2], Jiang Qu[3], Shuyu Wen[1], Ye Yuan[4], Slawomir Prucnal[1], Manfred Helm[1,2], Artur Erbe[1,2], Shengqiang Zhou[1], and Yonder Berencén[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01062, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, 01069, Germany — [4]Songshan Lake Materials Laboratory, Dongguan, Guangdong, 523808 China

Beyond being an excellent encapsulant and gate dielectric 2D material, hexagonal boron nitride (hBN) is significant in exploring the use for polarized photonics functionalities. Optically active defects in the h-BN are intriguing, serving not only to enable the optical readout of spins but also to function as quantum emitters that operate at room temperature. Furthermore, the creation of defects in hBN disrupts the symmetry of the lattice and induces an in-plane anisotropic crystal structure. Here, we will uncover intriguing in-plane anisotropic phenomena in Raman response and photoluminescence in 2D hBN subjected to ion irradiation. Leveraging this discovery, we seamlessly integrated the ion-irradiated hBN into room-temperature p-i-n Si detectors. Notably, the ion-irradiated hBN will serve as the polarized-sensitive layer, while Te hyperdoped silicon will facilitate infrared absorption. This hybrid structure highlights its potential as a polarized sensitive photodetector for the applications of image sensing and the ability of compatible with the CMOS process.

HL 36.29 Wed 18:00 Poster E

**Proximity-induced exchange field in a 2D magnet/graphene heterostructure detected by the anomalous Hall effect** — Maximilian Luka[1], •Stefan Peterhans[1], Matthias Kronseder[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Since the first observation of magnetic order in 2D materials in 2017, several groups have exploited the properties of these materials, opening up a new field in addition to the vast range of 2D crystals. Materials such as, e.g., $Cr_2Ge_2Te_6$ (CGT) can be used to induce magnetic properties in single or bilayer graphene due to the magnetic proximity effect. These magnetic exchange fields can be detected by measuring the anomalous Hall effect (AHE). We were able to observe the AHE in a graphene/CGT/hBN-heterostructure. This observation was supported by SQUID-measurements to show the temperature dependence of the magnetization of CGT and its effect on the strength of the AHE. To exclude a trivial stray field effect, we measured the magnetic stray field of several magnetic materials ($Fe_3GeTe_2$, CGT) with graphene Hall micromagnetometry, where the 2D magnet was not in direct contact with the graphene layer. The signal detected in this configuration was significantly weaker than the AHE in the proximity-coupled heterostructure, confirming the presence of a magnetic proximity effect.

HL 36.30 Wed 18:00 Poster E

**Exciton condensation in $TiSe_2$ detected by screening of single-layer $WSe_2$** — •Adrian Dewambrechies, Benjamin Weintrub, and Kirill Bolotin — Freie Universität Berlin, Germany

Two-dimensional materials and the recent progress in their manipulation have provided a platform to study highly correlated phenomena, a relevant case being the condensation of the excitons dominating their optical response. Recent advances show that the exciton properties, and their tunability in such systems, offer the observation of high temperature condensation, and allows the study of the crossover between different types of condensates including the Excitonic Insulator. However, a definitive proof of the exciton condensation and superfluidity is still missing mainly due to the charge of excitons being zero, and new experimental techniques are being explored in this direction. Here, we present our latest results in the detection of exciton condensation in two-dimentional semimetal $TiSe_2$. We study its effect in the dielectric environment of a nearby sensor layer of $WSe_2$, by tracking the emission and absorption of its excitons to understand charge transfer between the two materials and the potential transition to an excitonic insulating state in $TiSe_2$.

HL 36.31 Wed 18:00 Poster E

**Synthesis and properties of 2D Janus materials** — •Jens Osterfeld, Jennifer Schmeink, Osamah Kharsah, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Among two dimensional semiconductor materials, transition metal dichalcogenides (TMDCs), such as molybdenum disulfide, are studied the most. More recently, 2D Janus materials based on TMDCs were discovered. They can be created by exchanging one of the chalcogen layers in a base TMDC with another species of chalcogen atoms, thus forming an asymmetrical Janus structure with new, unique properties [1]. As the process selectively substitutes the top-most layer of chalcogen atoms with another kind, there is a likelihood of a partial substitution. In such instances the resulting material would resemble an alloy more closely than a Janus structure. These alloys consist of regions with different stoichiometry, which means they represent an ideal bridge between the characteristics of the base TMDC and the ideal Janus materials.

With my poster, I will showcase my latest achievements in synthesizing Janus materials and their alloys, and the characterization of their features with Raman and Photoluminescence spectroscopy.

[1] J. Schmeink *et al.*, Nanoscale (2023), **15**, 10834-10841

HL 36.32 Wed 18:00 Poster E

**Light induced dynamics in a coupled van der Waals heterostructure** — •Mashood Tariq Mir, Arne Ungeheuer, Ahmed Hassanien, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

Layered transition metal dichalcogenides (TMDs) host a rich collection of physical properties, opening many applications with atomically thin films such as sensors, electronic switching, or energy storage. Among those materials, 1T-TaS2 exhibits a complex phase diagram depending on temperature encompassing charge density waves (CDW) with diverse commensurabilities. New phenomena have been observed and are further expected from combining different materials to 2D heterojunctions. We employ the UED technique to investigate the light-induced dynamics in the sub-ps time regime. This work uses femtosecond laser pulses to induce rapid structural changes in a free-standing van der Waals heterostructure. Upon lattice heating, the CDW material undergoes several phase transitions. We focus on the reversible phase transition 1T-TaS2 from the nearly commensurate to the incommensurate phase. In addition, we present an initial UED study on the optically excited CAPs in a stacked (1T-TaS2 / Graphite) heterostructure.

HL 36.33 Wed 18:00 Poster E

**Coherent interlayer phonons in van der Waals MoSe2/WSe2 heterobilayers** — Changxiu Li[1,2], Alexey V. Scherbakov[1], •Pedro Soubelet[3], Anton K. Samusev[1], Claudia Ruppert[1], Nilanthy Balakrishnan[4], Vitalyi E. Gusev[2], Andreas V. Stier[3], Jonathan J. Finley[3], Manfred Bayer[1], and Andrey V. Akimov[5] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Germany. — [2]Laboratoire d'Acoustique de l'Université du Mans, Institut d'Acoustique-Graduate School, Le Mans Université, France. — [3]Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Germany. — [4]School of Chemical and Physical Sciences, Keele University, United Kingdom. — [5]School of Physics and Astronomy, University of Nottingham, United Kingdom.

The increasing role of two-dimensional (2D) devices requires the development of new techniques for ultrafast control. A special feature of heterobilayers (HBs) assembled from van der Waals (vdW) monolayers is the femtosecond separation of photoexcited electrons and holes between the neighboring layers, resulting in the formation of Coulomb forces. Using laser pulses, we generate a 0.8THz coherent breathing mode in MoSe2/WSe2 HBs, which modulates the thickness of the HB and should modulate the photogenerated electric field in the vdW gap. While the phonon frequency and decay time are independent of the stacking angle between monolayers, the amplitude decreases at intermediate angles, which is explained by a decrease in the photogenerated electric field between the layers.

HL 36.34 Wed 18:00 Poster E

**Layered Minerals and Chalcogenides investigated by Atom Probe Tomography** — •Jan Köttgen[1], Alexander Kiehn[2], Anna Vymazalová[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]1. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Institute "Green IT (PGI-10)", Forschungszentrum Jülich, 52428 Jülich, Germany — [3]Czech Geological Survey, Geologická 6, 152 00, Prague, Czech Republic

Layered solids have recently attracted considerable attention due to the vast range of properties that can be realized in such layered systems. Layered chalcogenide compounds, in particular, exhibit a rich variety of structures. Some of these materials also employ metavalent bonding, which is a distinctive bonding mechanism initially discovered in crystalline phase change materials (PCM). The bonding between the atoms can be investigated by breaking these bonds in atom probe tomography. Compounds such as GeTe or $Sb_2Te_3$ exhibit unconventional properties indicative for the presence of metavalent bonding e.g. typically one electron per bond shared between atoms, and a high probability of multiple events observed in atom probe tomography. The aim of this project is to better understand the relation between layered solids and metavalent bonding, focusing on the transition metal chalcogenides $PdTe_2$ and $Pt_3Te_4$, and comparing them with layered minerals like vihorlatite ($Bi_{24}Se_{17}Te_4$). All layered systems investigated exhibit a high multiplicity during laser-assisted atom probe tomography, indicative for an unusual bonding mechanism. Further experiments will be presented which help to classify and understand these layered solids.

HL 36.35 Wed 18:00 Poster E

**Size Dependence of Electrical Properties of Thin Film $ZrSe_3$** — •Davin Höllmann[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

Among the popular group of transition metal chalcogenides, the transition metal trichalcogenides show unique properties, such as a quasi-1D structure [1]. Previous work displayed different electrical properties of $ZrSe_3$ [2]. Building on this, the influence of the sample geometry on the electrical properties of thin film $ZrSe_3$ was investigated. The bulk material used was fabricated by a chemical vapor transport method and then exfoliated to achieve thin films.

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, an unusual width dependence of the conductivity in thin $ZrSe_3$ was found. By comparing the widths and conductivities of wide and narrow samples, a non-linear increase in the conductivity ratio with increasing width ratio was observed.

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

HL 36.36 Wed 18:00 Poster E

**Realizing thermoelectric transport measurements in dual-gated Bernal bilayer graphene** — •Moritz Knaak, Martin Statz, and Thomas Weitz — University of Göttingen, Faculty of Physics, 1st Institute of Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In dual-gated, hexagonal boron nitride (hBN) encapsulated, trigonally warped Bernal bilayer graphene (BLG) many correlated phases at high out-of-plane electric fields have been found.[1-3]. They were found close to Lifshitz transitions, where the density of states(DoS) is high and which can be induced by tuning the out-of plane electric field or the charge carrier density. While conductance measurements alone only give an indirect probe of the DoS, in thermoelectric transport measurements we can study the Seebeck coefficient, which provides a more direct probe of it. To measure the Seebeck coefficient, we use an on-chip heater next to the hBN-encapsulated BLG which is dual-gated and contacted by graphite gates and contacts. The source-drain contacts are simultaneously used as 4-point-probe on-chip resistance thermometers to determine the local temperature differences. A dry-transfer method, e-beam-lithography, reactive ion etching as well as thermal evaporation of contact leads are employed for the fabrication of the thermoelectric devices.

[1] Seiler, A.M. et al. Nature 608, 298-302 (2022) [2] Zhou, H. et al. Science 375, 774-778 (2022) [3] de la Barrera, S. C. et al. Nat. Phys. 18, 771-775 (2022)

HL 36.37 Wed 18:00 Poster E

**Optical spectroscopy of atomically thin $MoS_2$ under high pressure** — •Paul Steeger, Jan-Hauke Graalmann, Robert Schmidt, Philipp Marauhn, Marie-Christin Heissenbüttel, Jan Nellesen, Ilya Kupenko, Carmen Sanchez-Valle, Steffen Michaelis de Vasconcellos, Miachel Rohlfing, and Rudolf Bratschitsch — University of Münster, Germany

High-pressure diamond anvil cells (DACs) are a recent addition to the toolkit for investigating two-dimensional materials and their heterostructures. They can exert compressive strain to samples, allowing precise manipulation of interlayer coupling strength in multi-layered van der Waals materials. Here, we present pressure-dependent optical transmission spectra of 2H-$MoS_2$ bilayers under pressure and extract the respective energy shift rates of inter- and intralayer excitons. Additionally, our findings highlight an interesting observation: the actual deformation of the sample differs from hydrostatic compression due to substrate effects. We discuss strategies to address this common challenge encountered in high-pressure experiments on 2D materials in conjunction with complementary DFT-based calculations. [1]

[1] P. Steeger, J.-H. Graalmann et al., Nano Lett., 23, (2023)

HL 36.38 Wed 18:00 Poster E

**Cryogenic nano-imaging of the metal to charge density wave transition in NbSe2** — •Monica Kolek Martinez de Azagra, Francesca Falorsi, Christian Eckel, and Thomas Weitz —

Georg-August-Universität Göttingen

The transition metal dichalcogenide (TMDC) NbSe2 exhibits a metallic, charge density wave (CDW) - the periodic modulation of electron densities and lattice atoms - and a superconducting phase. The transition between these phases can be tuned by temperature variation. Previous studies have shown that the critical temperatures TCDW for the CDW transition and TC for the superconductivity are layer dependent. While calculations have shown that with decreasing layer thickness the CDW order is enhanced with a gain in energy [1], experimental results contradict each other regarding the TCDW for few-layer and bulk NbSe2. [2,3] Here, we present our preliminary results on the investigation of 2H-NbSe2 using a cryogenic scanning near-field microscope (SNOM), to image the layer-dependent TCDW. Using SNOM we are able to provide real-space images while probing the dielectric function of the NbSe2 few-layer flakes with nanometer resolution. Subsequently, we will be able to verify our results using transport measurements in situ.

HL 36.39 Wed 18:00 Poster E

**Optimization of magnetic topological insulators by magneto-transport measurements** — •Jonas Buchhorn[1,2], Jan Karthein[1,2], Kaycee Underwood[1,2], Abdur Rehman Jalil[1,2], Michael Schleenvoigt[1,2], Peter Schüffelgen[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich und RWTH Aachen University, 52425 Jülich, Germany

Edge channels in magnetic topological insulators in the quantum anomalous Hall state are a promising platform for quantum computing, when they are in proximity to a superconductor. Majorana modes are proposed to emerge which by non-abelian braiding statistics lead to a fault-tolerant computing paradigm. In this work, probing the chiral edge channels in Cr-doped $(Bi_xSb_{1-x})_2Te_3$ thin films is shown together with other properties of this material system that are observable by quasi DC magneto-transport measurements in Hall bars at cryogenic temperatures. A time-efficient feedback loop between electrical measurements and molecular beam epitaxy was established to investigate the impact of growth parameters on the magneto-transport properties of the thin films with minimal fabrication. The results of the feedback loop are presented and, together with the findings of the Hall bar measurements, they lead to a guideline on how to tune the magnetic topological insulator into the bulk- and surface-insulating regime, isolating the chiral edge channels from residual conductance.

HL 36.40 Wed 18:00 Poster E

**Efforts to make Josephson junction on a quantum anomalous Hall insulator** — •Bibek Bhujel[1], Anjana Uday[1], Gertjan Lippertz[1,2], Kristof Moors[3], Henry F. Legg[4], Andrea Bliesener[1], Lino M. C. Pereira[2], Alexey A. Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany — [2]KU Leuven, Quantum Solid State Physics, Celestijnenlaan 200 D, 3001 Leuven, Belgium — [3]Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, 52425 Jülich, Germany — [4]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Recently, we obtained evidence for superconducting pair correlation in the chiral edge states of a vanadium-doped $(Bi_xSb_{1-x})_2Te_3$ thin film that is tuned to the quantum anomalous Hall insulator phase, by observing the negative nonlocal resistance downstream from a narrow superconducting (grounded) Nb finger electrode [1]. This negative downstream resistance is due to the crossed Andreev reflection (CAR) process, which creates superconducting correlations in the chiral edge. To further investigate the superconducting proximity effect, we are currently fabricating Josephson junction on QAHI. This is a difficult experiment because the 2D "bulk" of the QAHI is insulating and the ferromagnetism works against superconductivity. We will report the progress we have made so far by using Nb electrodes.

[1] A. Uday et al., arXiv:2307.14196

HL 36.41 Wed 18:00 Poster E

**Thermal anisotropy of $\beta - Ga_2O_3$ on ultra-short length scales** — Moritz Meissner[1], •Luca Sung-Min Choi[1], Alwin Wüthrich[1], Kai Xu[2], Riccardo Mincigrucci[3], Laura Foglia[3], Danny Fainozzi[3], Filippo Bencivenga[3], Sebastian Reparaz[2], and Markus R. Wagner[1,4] — [1]Technische Universität Berlin, Berlin, Germany — [2]Institut de Ciència de Materials de Barcelona, Barcelona, Spain — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The monoclinic beta-phase of gallium oxide, known for its ultra-wide bandgap, emerges as a promising candidate for power electronic device technologies. We examine whether the macroscopic thermal anisotropy persists on the nanoscale. Employing the optical transient thermal grating (TTG) method, we determine the in-plane anisotropy of thermal transport and acoustic phonons across different grating length scales ranging from 110 to 26 nm. Thereby examining potential length-scale dependencies of the $\beta - Ga_2O_3$ anisotropy. Our experiments, conducted at the Fermi Free Electron Laser (FEL) [Elettra Synchrotron Trieste, dedicated endstation EIS-TIMER] on a (001)-$\beta - Ga_2O_3$ sample, enable the observation of thermal effects at ultra-short length scales.

HL 36.42 Wed 18:00 Poster E

**Thermal Conductivities of Crystalline Polymers calculated with Machine-Learned Potentials** — •Lukas Reicht, Lukas Legenstein, Sandro Wieser, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Disordered polymers are typically characterized by a very low thermal conductivity on the order of 0.1 W/mK. In contrast, recent experiments showed that, when polymers are highly aligned (crystalline), polyethylene (PE) can reach a thermal conductivity of ˜104 W/mK, which would be interesting for applications. Newly developed machine-learned potentials (MLP) promise to be an efficient and accurate tool for calculating these thermal conductivities. Applying a new methodology, however, requires a thorough benchmarking. We performed such a benchmarking for moment tensor potentials (MTPs), which are a flavour of machine-learned potential, by calculating various phonon related properties of polyethylene (PE), polythiophene (PT), and poly(3-hexyl-thiophene) (P3HT). Based on the calculated phonon band-structures, elastic constants, thermal expansion coefficients, and thermal conductivities, we conclude that the accuracy of MTPs can be substantially increased by a deliberate choice of training data adapted to the intended use case. Having established the accuracy of the trained MTPs, they are used to calculate thermal conductivities of PE and PT using the Boltzmann transport equation (BTE), non-equilibrium molecular dynamics (NEMD), and the approach-to-equilibrium molecular dynamics (AEMD). This provides complementary atomistic insights into the factors determining heat transport.

HL 36.43 Wed 18:00 Poster E

**Phonon Bands and Thermal Conductivities of Organic Semiconductors using Machine-Learned Moment Tensor Potentials** — •Lukas Legenstein[1], Lukas Reicht[1], Sandro Wieser[1], Michele Simoncelli[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]TCM Group, Cavendish Laboratory, University of Cambridge, UK

Phonons affect transport properties in crystalline organic semiconductors either by scattering with charge carriers, or as the main carriers of thermal energy. Modelling these phonons and their transport gives a distinct advantage of providing direct insight into the relevant processes at an atomistic level compared to experiments. Of particular relevance for such simulations are machine-learned potentials, which often achieve accuracies comparable to the ab initio methods they are trained on, albeit at hugely reduced computational costs. In this work we use Moment Tensor Potentials (MTP) to determine the phonon properties of the acenes (from benzene to pentacene). We show that the MTPs excellently reproduce the phonon bands calculated previously using dispersion-corrected density-functional theory. Further, we determine the lattice thermal conductivity by solving the Wigner transport equation. With this methodology the conduction mechanisms arising from inter-band tunneling are accounted, which turns out to be crucial for matching the temperature-dependent experimental values for naphthalene and anthracene. Importantly, the presented approach provides direct insight into the (anisotropic) contributions of individual modes to the thermal conductivities.

HL 36.44 Wed 18:00 Poster E

**Nitrogen-doped Ni-TiO2 Nanoarrays via plasma treatment as Sodium-Ion Battery Anodes** — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-ion batteries (SIBs) are a potential substitute for Li-ion batteries for energy storage devices due to their abundant reserves and low sodium cost. TiO2 is considered one of the promising anodes for SIBs due to its large sodium storage capacity. However, low electrical conductivity greatly reduces its rate performance and limits the broad application of TiO2 for SIBs. Here, we fabricated 3D Ni-TiO2 core-shell nanoarrays using nanoimprinted AAO templating and atomic layer deposition (ALD) technique. Then, the 3D Ni-TiO2 nanoarrays were treated via a nitrogen plasma system and directly used as anode. The 3D Ni-TiO2 arrayed anode can offer fast electron transport and high ion accessibility, and the nitrogen-doping also significantly improves the electrical conductivity of TiO2, resulting in a significant enhancement of the electrochemical performance, especially the rate performance.

HL 36.45 Wed 18:00 Poster E

**Energy landscape around the $B_{Si}Si_i$ defect - a DFT Study** — •Aaron Flötotto[1], Wichard J. D. Beenken[1], Kevin Lauer[1,2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is an important dopant of silicon. It often forms the so-called $B_{Si}Si_i$ defect, which has been suggested as a source of light-induced degradation (LiD) in solar cells made from boron-doped Czochralski-grown silicon [1]. In this study, we calculated the energy landscape around the $B_{Si}Si_i$ defect by first principle methods. This includes also configurations with only one interstitial B atom as well as a B–Si pair sharing a vacancy in the lattice. Between the meta-stable defect configurations we identified minimal energy paths utilizing the Nudged Elastic Band method. The resulting potential energy landscape is compared with previous models for boron diffusion and LiD. For the latter we identified possible recombination centers among the meta-stable defect configurations by their electronic DOS.

HL 36.46 Wed 18:00 Poster E

**High-performance aqueous zinc-ion batteries based on the three dimensional manganese vanadate nanoflower cathode** — •Yan Ran[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

In this work,manganese vanadate(MnVO) synthesized via a one-step hydrothermal method is proposed as a promising cathode material for AZIBs. Because the stable layered structure and hieratical morphology of MnVO provide a large layer space for rapid ion transports, this material exhibits high specific capacity (433 mAh g-1 at 0.1 A g-1), an outstanding long-term cyclability (5000 cycles at a current density of 3 A g-1), and an excellent energy density. To illustrate the intercalation mechanism, ex situ X-Ray diffraction, Fourier transform infrared spectroscopy, and X-ray photo-electron spectroscopy are adopted, uncovering an H+/Zn2+ dual-cation co-intercalation processes. In addition, density-functional theory calculation analysis shows that MnVO has a delocalized electron cloud and the diffusion energy barrier of Zn2+ in MnVO is low, which promotes the Zn2+ transport and consequently improves the reversibility of the battery upon deep cycling. The key and enlightening insights are provided in the results for designing high-performance vanadium-oxide-based cathode materials for aqueous zinc ion batteries.

HL 36.47 Wed 18:00 Poster E

**High-performance aqueous zinc-ion batteries based on the three dimensional manganese vanadate nanoflower cathode** — •Yan Ran[1], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

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HL 36.48 Wed 18:00 Poster E

**Structural reconfiguration of Bi(111) thin layers upon Na intercalation** — •Peter Markmann, Uwe Gerstmann, Wolf Gero Schmidt, Guido Grundmeier, and Adriana Bocchini — Paderborn University, Warbuger Str. 100, 33098 Paderborn

Current technologies for energy storage are mainly based on lithium-ion batteries. Due to the low abundance of Li in the earth crust, other elements, e.g. heaviear alkali ions like sodium have to be considered for near future technology, but require well-adapted material for the electrodes.

In this work, with the help of DFT calculations, we investigate Bi(111) thin layers as a possible candidate. We show that the material in fact allows for interacalation of Na atoms in high concentrations up to 50 %, whereby the volume expansion is moderate and limited to the direction perpendicular to the Bi bilayers. Interestingly, if local concentration reaches atomic ratios of 1:2, a structural reconfiguration takes place, characterized by the appearance of 35°-tilted fractions of Bi-bilayers. Notably and in contrast to oxidization, this structural phase transitions is fully reversible under Na deintercalation and further reduces the volume expansion.

HL 36.49 Wed 18:00 Poster E

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HL 36.50 Wed 18:00 Poster E

**Accurate computational description of electronic and structural properties of bismuth vanadate** — •Philip Schwinghammer, Frederico Delgado, Franziska Hegner, 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 density functionals did not correctly reproduce the ground state geometry 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. In addition, we also found the electronic properties to depend significantly on the inclusion of spin-orbit coupling. Particularly the states near the valence band edge have a profound impact on the monoclinic distortion, indicating that a reliable description of BVO is only possible when fully accounting for the relativistic effects due the heavy bismuth ions and using hybrid functionals.

HL 36.51 Wed 18:00 Poster E

**Electrochemical properties of F-doped $RbTiOPO_4$ (RTP:F) predicted from first principles** — •Yingjie Xie, Uwe Gerst-

mann, Wolf Gero Schmidt, and Adriana Bocchini — Universität Paderborn, 33095 Paderborn, Germany

Battery technologies based on heavier alkali ions are considered promising candidates to substitute for current Li-based technologies. However, due to the larger ionic radii, new electrode materials are required to guarantee, e.g., high energy densities, a fast ion (de)intercalation, and a robust long-term operation. In this context, many recent studies suggest the potassium titanyl phosphate ($KTiOPO_4$, KTP) crystals as promising electrodes in alkali-ion batteries [1-4].

Here, we characterize the structural properties of a novel KTP-type material, i.e., $RbTiPO_4F$ (RTP:F), and discuss its electrochemical performance for Rb-ion batteries (RIBs) using density functional theory (DFT). The material shows promising electrochemical properties for cathode application: A rather high average voltages of more than 2.8 V and a modest volume shrinkage of less than 13% are predicted upon the deintercalation of Rb.

[1] Fedotov et al., Chem. Mater. 26, 411 (2016)
[2] Fedotov et al., J. Mater. Chem. 6, 14420 (2018)
[3] Huang et al., J. Phys. Lett. 12, 2721 (2021)
[4] Bocchini et al., Phys. Rev. Materials 6, 105401 (2022)

HL 36.52 Wed 18:00 Poster E

**Atomic Layer Deposition of Pt-doped $Ta_2O_5$ Coatings for Photoelectrochemical Water Splitting** — •Julius Kleusberg[1,2], Tim Rieth[1,2], Guanda Zhou[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]TUM School of Natural Sciences, TU Munich, Garching, Germany

Photoelectrochemical (PEC) water splitting provides a promising avenue for transitioning from a fossil fuel-based economy towards low-carbon alternatives. In PEC devices, photoabsorbers are immersed into an electrolyte, absorb light, generate and separate electron-hole pairs, and thereby drive the water splitting reactions. However, the chemical instability of many efficient photoabsorbers under PEC conditions remains a critical challenge. Consequently, a quest for functional coatings protecting the photoabsorber arise. Tantalum oxide ($Ta_2O_5$) emerged as promising protective material due to its high electrochemical inertness and full transparency to the solar spectrum. However, as wide bandgap semiconductor, $Ta_2O_5$ suffers from low electrical conductivity that prevents efficient charge transport to the catalytic surface. In this study, we introduce Pt sub-cycles in a $Ta_2O_5$ ALD process to achieve Pt-doped $Ta_2O_5$ thin films with enhanced electrical conductivity. We tailor the Pt-concentration via the sub-cycle ratio and thereby introduce additional states at the valance band edge that shift the Fermi-level downwards. Finally, we apply the developed Pt-doped $Ta_2O_5$ coatings on $BiVO_4$ photoanodes, analyse PEC improvements, and, ultimately, demonstrate doped ALD coatings as a promising way towards durable photoelectrochemical water splitting.

HL 36.53 Wed 18:00 Poster E

**Exploring spin-dependent transport in $BiVO_4$** — •Sven Doll, Melina Pees, David Vogl A., Noah Braitsch, Ian D. Sharp, and Martin S. Brandt — Walter Schottky Institut and School of Natural Sciences, Technische Universität München, 85748 Garching, Germany

Bismuth vanadate $BiVO_4$ is a promising photoanode material for solar-to-fuel conversion. This semiconductor is particularly interesting considering its strong visible light absorption, efficient charge carrier separation, and favorable quasi-Fermi-level alignment with relevant redox potentials. However, small polaron transport strongly reduces its performance. To gain further insight into the charge carrier transport by these polaronic states, we explore whether we can observe a spin dependence of the hopping of the small polarons in $BiVO_4$ using electrically detected magnetic resonance (EDMR). We investigate polycrystalline thin films grown by metal-organic decomposition on conductive and non-conductive transparent substrates. Furthermore, we prepared different electrical contact configurations via physical vapor deposition to analyze in-plane and out-of-plane transport in this material and to achieve small resistances and RC time constants to meet the experimental requirements of EDMR. Since spin-dependent signals are known to critically depend on the charge carrier density (e.g., from similar experiments on doped crystalline silicon), we evaluate the possibility of using the persistent photoconductivity of $BiVO_4$, as well as the introduction of donors in the form of oxygen vacancies and hydrogen impurities, to tune the polaron density.

HL 36.54 Wed 18:00 Poster E

**Photoelectrochemical $CO_2$ reduction with co-catalysts on atomic layer deposited titania protection layers** — •Giovanni Postacchini[1,2], Julius Kühne[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Light-driven $CO_2$ reduction is a promising approach to sustainably address increasing anthropogenic $CO_2$ emissions and meet the ever-increasing energy demand through the production of solar fuels. However, in an electrochemical environment, the semiconductor photoabsorber must be chemically protected against harsh reaction conditions. Atomic layer deposited (ALD) titania is an optimal candidate for photocathode corrosion protection layers thanks to its chemical stability, passivating effect, and optical transparency in the visible/infrared spectrum. Here, different Ag co-catalyst thin layers are deposited on titania-protected photoabsorbers. The photocathodes are characterized by photoelectrochemical (PEC) measurements using a three-electrode setup in a two-compartment cell to assess the photoelectrocatalytic activity and stability under $CO_2$ reduction conditions. Gas chromatography (GC) measurements allow the quantification of the product gases and determination of the selectivities of photoanodes towards desired reaction products. Further ex-situ AFM, SEM and XPS analyses are conducted to study surface morphology and composition changes and to elucidate possible degradation mechanisms.

HL 36.55 Wed 18:00 Poster E

**Challenges in optical detection of high-amplitude deflections of micro- and nanomechanical systems** — •Jannik Dornseiff, Mengqi Fu, Fan Yang, and Elke Scheer — Universität Konstanz, Deutschland

Micro-electro-mechanical systems (MEMS) and their behavior in the nonlinear, high amplitude regime have gathered great interest for research as well as for many engineering applications, like signal processing [1] and amplification [2], mass sensing [3], displacement measurement [4] and more. Optical detection methods, like digital holography microscopy (DHM) or Michelson interferom- etry are versatile and efficient methods of investigating MEMS, but they come with challenges, particularly when it comes to the calibration of the deflection amplitude [5]. By comparison of the results obtained with different instruments, acquisition schemes and analysis methods [6, 7] we are able to identify artifacts, arising from the nonlinear optical transduction when the deflection amplitude overcomes a certain fraction of the optical wavelength used for the detection. We give several examples and also discuss mitigation strategies to minimize these artifacts.

[1] Erbe A et al Appl. Phys. Lett. 77 3102-4 (2000); [2] Almog R et al Appl. Phys. Lett. 88 213509 (2006); [3] Buks E and Yurke B Phys. Rev. E 74 046619 (2006); [4] Trusov A and Shkel A J. Micromech. Microeng. 17 1583-92 (2007); [5] Dolleman RJ et al Appl. Phys. Lett. 111 253104 (2017);[6] Waitz R et al Phys. Rev. B 85 035324 (2012); [7] Yang F et al Sensors and Actuators A: Phys. 354 114307 (2023)

HL 36.56 Wed 18:00 Poster E

**Enhancement of wurtzite AlN by ion beam strain engineering: experiments and simulations** — •Florian Fuchs[1,2], Holger Fiedler[3], John V. Kennedy[3], and Jörg Schuster[1,2] — [1]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [3]National Isotope Centre, GNS Science, Lower Hutt, New Zealand

We study the piezoelectric properties of wurtzite AlN, and in particular the enhancement of these properties by noble gas [1] and transition metal interstitials.

Using ion-beam implementation, Ne, Ar, Xe, Ti, Zr, and Hf ions were implanted. The measurements show a massive increase in the $d_{33}$ component of the piezoelectric tensor of up to 30% when using $Ar^+$ or $Ti^+$. Scanning transmission electron microscopy was utilized to characterize the underlying structure after ion-implantation, demonstrating the occurrence of different interstitial types and the formation of chemically inaccessible noble-gas containing materials.

Density functional theory was used to calculate formation energies of the noble gas interstitials, showing that larger noble gases require a larger formation energy. The most stable positions of the interstitial within the AlN lattice were also determined. Finally, the piezoelectric tensor was calculated and compared to the experimental measurements.

[1] H. Fiedler et al., *Adv. Electron. Mater.* **7**, 2100358 (2021)

HL 36.57 Wed 18:00 Poster E

**Theoretical Study on the Cubic (In, Ga)N Random Alloy and Ordered Structures** — •Christian Maas[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

Through variation in the composition $x$ of indium gallium nitride $In_xGa_{1-x}N$, the band gap can be engineered over the full visible spectrum. By utilizing the cubic zincblende structure, the presence of polarization fields can be avoided intrinsically. Otherwise, these fields could have a negative impact on certain properties, for instance the efficiency of LEDs.

In general, (In,Ga)N is a random alloy, even though there are recent reports on an CuPt-type ordering at certain compositions. We apply the coherent potential approximation (CPA)[1] to describe the random alloy for any given composition. To properly predict the fundamental electronic band gap, we use the low computational cost LDA-1/2 method [2]. In this study, we present our results on structural and electronic properties such as stability, lattice parameter, band gap and phonon modes for the random alloy and certain ordered structures such as the CuPt-type ordering.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). https://doi.org/10.1103/PhysRevB.88.094421

[2] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). https://doi.org/10.1103/PhysRevB.78.125116

HL 36.58 Wed 18:00 Poster E

**Temperature dependent free carrier concentration in GaN:Si** — •Christina Harms, Jona Grümbel, Rüdiger Goldhahn, and Martin Feneberg — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany

GaN is already commercialized in a variety of different applications. Nevertheless, still fundamental questions remain to be answered. Here, we focus on the temperature dependence of the free carrier concentration of doped GaN. We investigate the Raman excitations of hexagonal bulk GaN:Si from 80 K to 300 K. Six samples with carrier concentrations ranging from $10^{12}$ to $10^{19}$ $cm^{-3}$ were measured using laser excitation at 532 nm. Our results reveal that at room temperature, both coupled phonon-plasmon modes ($LPP_{\pm}$) are visible and agree with Hall-effect experiments. Under temperature variation, the $LPP_+$ mode shows a weak frequency shift or remains even unaffected. Surprisingly, the $LPP_-$ mode exhibits a frequency shift towards higher frequencies with decreasing temperatures for all samples, contradicting previous assumptions. To shed light onto this shift, photoluminescence spectra are taken into account as well. The combination of both experimental data sets allows to better understand the evolution of temperature dependence of the free carrier concentration.

HL 36.59 Wed 18:00 Poster E

**Electrical characterization of n-GaN nanowires to n-Si(111) growth substrates with AlN interlayer** — •Juliane Koch[1], Patrick Häuser[2], Peter Kleinschmidt[1], Werner Prost[2], Nils Weimann[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]University of Duisburg-Essen, Components for High Frequency Electronics (BHE), Duisburg, Germany

III-V semiconductor nanowires (NW) have demonstrated high potential as building blocks in a wide range of applications in electronic and optoelectronic devices. In particular, GaN-based nanowires have attracted attention in recent years, especially in the field of UV-LEDs and sensors. For the realization of these devices, special attention must be paid to the surfaces and interfaces, since the electrical properties can be strongly influenced by the surface properties and the sequence of layer deposition. A detailed electrical investigation is therefore necessary, which was done by a four-point measurement method using a multi-tip scanning tunnelling microscopy (MT-STM). For this purpose, we investigate in this work single GaN NWs in an upright standing configuration applying a MT-STM and a built-in scanning electron microscope. We focus on the limiting factors of the current in GaN NWs on an n-doped Si(111) substrate. Our detailed investigations reveal the NWs themselves are highly conductive and that the NW-to-substrate junction as the limiting factor, dominating the overall electrical behavior. The impact of the junction is strongly dependent on the thickness and crystal structure of the AlN layer.

HL 36.60 Wed 18:00 Poster E

**Atomic structure of As-modified Si(100) surfaces prepared in MOCVD ambience utilizing background arsenic** — Chris Yannick Bohlemann[1], Agnieszka Paszuk[1], Manali Nandy[1], Aaron Flötotto[2,3], Max Grossmann[2,3], Oleksandr Romanyuk[4], •Kai Daniel Hanke[1], Peter Kleinschmidt[1], Erich Runge[2,3], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials — [2]TU Ilmenau, Institute of Physics,Theoretical Physics I — [3]TU Ilmenau, Centre of Micro- and Nanotechnologies — [4]Institute of Physics, Academy of Sciences of the Czech Republic, 182 00 Prague 8

A low-defect III-V nucleation layer and a well-defined atomically abrupt interface between the Si(100) substrate and the III-V nucleation layer are essential prerequisites for subsequent low-defect III-V layer growth. Preparation of a well-ordered Si(100) surface in industrially-relevant MOCVD ambience with arsenic benefits in a significant temperature reduction during the deoxidation step. In this study, we investigate the atomic structure of Si(100) surfaces prepared in As-rich MOCVD reactor, employing background arsenic as the arsenic source. The preparation of the samples in the MOCVD reactor was monitored in situ by surface sensitive optical spectroscopy and the surfaces were characterized in UHV by FTIR and STM. The measurements are supported by complementary DFT calculations. We confirm presence of hydrogen on the surface and mixed As-Si-H dimers, which was previously unrecognized.

# HL 37: Poster IV

Topics:
- Materials and devices for quantum technology
- Nitrides
- Semiconductor lasers
- Transport properties of semiconductors
- Ultra-fast phenomena

Time: Wednesday 18:00–20:30 Location: Poster F

HL 37.1 Wed 18:00 Poster F

**SignalSnap and QuantumCatch: Python Libraries for Analyzing General Quantum Measurement Records** — •Markus Sifft and Daniel Hägele — Ruhr Uni. Bochum, DE

Quantum measurement records exhibit diverse characteristics ranging from Gaussian noise to telegraph noise and even to clicks at random times. Traditional evaluation methods often cater to one of those noise characteristics, while general methods especially for intermediate regimes are missing. We close this gap by analyzing measurements in terms of their higher-order temporal correlations that are directly related to the Liouvillian of the measured quantum system.

This approach is made readily available by two Python libraries: SignalSnap [1] and QuantumCatch [2]. SignalSnap computes higher-order correlations of the detector output, while QuantumCatch relates them to the Liouvillian of the measured quantum system. Higher order correlations follow from the stochastic master equation covering coherent quantum dynamics, environmental damping, and measurement backaction at arbitrary measurement strength. Using SignalSnap and QuantumCatch quantum measurements were evaluated from the realms of conventional spin noise spectroscopy [3], quantum transport experiments [4], and ultra-weak measurements with stochastically arriving single photons [5,6].

[1] github.com/markussifft/signalsnap, [2] github.com/markussifft /quantumcatch, [3] Hägele PRB 98, 205143, [4] Sifft PRR 3, 033123, [5] Sifft PRA 107, 052203, [6] Sifft arXiv:2310.10464

HL 37.2 Wed 18:00 Poster F

**Photoluminescence studies of erbium implanted GaAs nanostructures** — •Nico Brosda[1], Christian Düputell[1], Natalie Jung[2], Lisa Kreuzer[2], Nils C. Gerhardt[2], Martin R. Hofmann[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität-Bochum — [2]Lehrstuhl für Photonik und Terahertztechnologie, Ruhr-Universität Bochum

The rare earth element erbium emits light in the wavelength range of around 1.54 $\mu$m; this coincides with the absolute absorption minimum of optical fibres in the so-called C-band. Molecular beam epitaxial grown GaAs was used as a semiconductor matrix for erbium; the implantation was carried out with the help of a focused ion beam system at ion energies around 250 keV. Due to the damage to the crystal structure, thermal annealing is necessary. Utilizing photoluminescence (PL) measurements, statements about optimal parameters and dependencies can be made.

The recorded PL spectra at different implantation and annealing parameters were compared. A temperature range of 700 °C to 800 °C and implantation into 300 °C hot samples was particularly advantageous for maximum erbium luminescence. Furthermore, a temperature-induced quenching of erbium luminescence was observed with a simultaneous increase in peak widths. Implantation of $Er_2O_3$ significantly increased the total intensity. By correlating PL lines with optical transitions in different crystal field symmetries, it can be concluded that different erbium centres are present in various crystal field symmetries.

HL 37.3 Wed 18:00 Poster F

**Real-Time Quantum Measurement Analysis with Polyspectra at up to 25 MHz Sampling Rates** — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Phyiscs adn Astronomy, Experimental Physics VI, Germany

Our research focuses on applying quantum polyspectra to analyze continuous quantum measurement records across weak, strong, and single photon regimes. We employ our Python library, SignalSnap [1], which leverages the ArrayFire library for accelerated computations using both CUDA and OpenCL backends, providing hardware flexibility. This acceleration enables us to develop a new library for real-time evaluation of measurements. To digitize the data, we utilize PicoScope, a brand of PC Oscilloscopes. By combining the capabilities of an Nvidia 4090 graphics card and PicoScope 4000 Series, we successfully implement our new library for measurements currently with 25 MHz sampling rates. Real-time evaluation of measurements provides several key advantages for experimentalists. It allows for the immediate identification and correction of obvious errors in the experiment, such as drift, misalignment, or unwanted external noise.

[1] https://github.com/MarkusSifft/SignalSnap

HL 37.4 Wed 18:00 Poster F

**Semiconductor membrane transfer for circular bragg gratings fabrication** — •Juan Nicolas Claro Rodriguez, Dennis Deutsch, Hermann Kahle, Klaus D Jons, and Dirk Reuter — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn

Semiconductor quantum dots are promising candidates to fulfill the requirements on the emission properties. Newly developed InGaAs quantum dots grown on a InP substrate using MBE deposition [2] are interesting for long-distance communication as they emit in the telecom C-band, where standard optical fibers exhibit an absorption minimum. The lack of brightness can be tackled by embedding them into cavity structures, improving the indistinguishability of the photons and entanglement fidelity. Among the different cavity designs, hybrid circular Bragg gratings stand out for their high and broad-range photon collection efficiency together with their elevated Purcell factor. These characteristic features are achievable thanks to the addition of a backside mirror spaced by a transparent medium from the semiconductor membrane containing the quantum dot which allows the reflection of the backscattered photons to the collecting lens [3]. Here, we present a membrane transfer method, a crucial step for achieving the desired cavity configuration. It involves growing the backside mirror on top of the sample before transferring the layer structure onto a new carrier using a press-bonding device. Subsequently, the original InP substrate is removed by wet chemical etching with HCl to allow for posterior illumination of the quantum dots.

HL 37.5 Wed 18:00 Poster F

**Towards deterministic color centers in graphene-covered hexagonal boron nitride** — •Ataur Rahaman Bhuiyan, Hossein Ostovar, Robert Schmidt, Philipp Wiesener, Harry Mönig, Rudolf Bratschitsch, and Ursula Wurstbauer — University of Münster, Institute of Physics, Wilhelm-Klemm Str 10, 48149 Münster

Deterministic generation and control of single photon emitters are of importance for quantum information technology. Such single-photon emitters (SPEs) have recently been discovered in various two-dimensional materials. Their properties are strongly dependent on the host materials and differ e.g. between TMDCs or hBN but also if the emitters originate from defects, strain, or moiré-potentials in twisted structures [1]. In this work, we investigate the generation of defects in hexagonal boron nitride (hBN) covered by graphene with the vision to ion-implant color center functional at room temperature. In order to find a suitable parameter range during ion implantation, the sputtering yield in dependence on ion materials (i.e. argon and helium), acceleration voltage, target material combination, and thickness (depth profile) has been studied in details by thorough SRIM (Stopping and Range of Ions in Matter) simulations. Argon sputtering is guided by those simulations. Prior and after to sputtering the hetero stacks are characterized. In this poster we discussed the findings of our combined simulation and experimental work to implant color centers that are presumably carbon-based within couple of hBN layers [1]. [1] S. Michaelis de Vasconcellos et al. Physica status solidi b259, 2100566 (2022).

HL 37.6 Wed 18:00 Poster F

**Optimization of the direct bonding process for the manufacturing of GaAs/Si template** — •Micha Seidel[1], Ponraj Vijayan[1], Matthias Seibold[2], Jakob Hirlinger-Alexander[3], Michael Jetter[1], and Peter Michler[1] — [1]Universität Stuttgart, 70569 Stuttgart, Germany — [2]21S GmbH, 72654 Neckartenzlingen, Germany — [3]Universität Ulm, 89081 Ulm, Germany

Silicon photonics has gained increasing significance as it allows for high-density photonic integrated circuits (PICs). The limitation of silicon lies in its indirect band gap, leading to inefficient light sources. In contrast, III-V materials demonstrate exceptional light-emitting characteristics, making it promising to synergize the strengths of silicon and III-V materials. One way to integrate of III-V material onto silicon platform is to transfer a thin III-V membrane onto silicon through direct wafer bonding forming a III-V on silicon bonded template. The bonded template can then be used for the epitaxial regrowth of various III-V based optical structures. This integration approach overcomes the challenges of the conventional direct growth approach, such as the high-density threading dislocation and anti-phase domain which arises due to the large lattice mismatch and material polarity difference, respectively. In this contribution, we will report on the optimization of a direct bonding process for the fabrication of a GaAs/Si template. Different parameters including plasma treatment, chemical surface activation, cleaning procedure before bonding, annealing temperature after bonding, were investigated to analyze their influence on the robustness, particularly the thermal durability of the bonded template.

HL 37.7 Wed 18:00 Poster F

**Deterministically fabricated wavelength-tunable quantum dot device for interfacing with atomic vapor-based quantum memory** — •Avijit Barua[1], Ching-Wen Shih[1], Yuhui Yang[1], Chirag C. Palekar[1], Lucas Rickert[1], Benjamin Maass[2], Norman V. Ewald[2], Jin-Dong Song[3], Janik Wolters[2], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin, Hardenbergstr. 36, Berlin, Germany — [2]German Aerospace Center (DLR), Rutherfordstr. 2, Berlin, Germany — [3]Korea Institute of Science and Technology, Seoul, Republic of Korea

Semiconductor quantum dots (QDs) are extensively investigated as single-photon sources for applications in photonic quantum technology. Here, we develop bright and strain-tunable semiconductor QD single-photon sources at the Cs-D1 transition wavelength (894.6 nm). The devices are designed and numerically optimized to maximize extraction efficiency using the finite element method. By considering circular Bragg resonators with integrated QDs and Au-backside mirror we theoretically expect a photon extraction efficiency over 90% and a Purcell factor of 0.07. In the device fabrication, we implement in-situ electron-beam lithography to integrate QDs with spatial precision as good as 20 nm to create bright single-photon sources. By means of photon autocorrelation measurements, we demonstrate single-photon purity up to 97%. Furthermore, we explore the prospects of interfacing the QD single photons with a room-temperature ladder-type atomic vapor-based memory that allows for low-noise storage and retrieval at high repetition rates.

HL 37.8 Wed 18:00 Poster F

**Towards an Open-Tunable Fiber Cavity for Enhanced Directionality in Single Photon Emission** — •Paul Steinmann[1], Stefan Linden[1], and Beata Kardynal[2] — [1]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany — [2]PGI-9, Forschungszentrum Jülich, Jülich, Germany

Advancements in quantum communication technologies demand the development of robust single photon sources. Indium-Arsenide quantum dots, which act akin to atomic systems, have been recognized as a bright source for single photons of high quality. These quantum dots, situated in high refractive index GaAs, typically exhibit non-directional photon emission, making their integration into optical fibers for practical applications challenging. We propose and implement an open-tunable fiber micro cavity as a solution to this challenge. Our approach involves the careful construction of a cryostat insert, ensuring mechanical stability under low-temperature conditions. This cavity enhances the rate and directionality of single photon emission, allowing for efficient photon generation and direct coupling into optical fibers. The design and construction of this fiber cavity are focused on stability and minimizing photon loss, thereby optimizing the efficiency of single photon sources for quantum technologies.

HL 37.9 Wed 18:00 Poster F

**Simulation of statistical electric field fluctuations in 28-Si:P** — •Finja Tadge, Nico Eggeling, Jens Hübner, and Michael Oestreich — Leibniz Universität Hannover, Germany

In this work, statistical electric field fluctuations are examined using the Monte-Carlo method to simulate the linewidth of the $D^0X$ excitonic transition in ultra-pure isotopically enriched 28-Si:P. The electric field inside a solid-state matrix is modelled with the help of a random distribution of ionized donors and acceptors as it would occur at temperatures around 4K. Distribution functions describing both the radius between ionized donors and acceptors and the electric field can be deduced. Using the Thomas-Fermi-Approximation the electric field distribution influencing optically active centres can be calculated. Furthermore, it is shown, that the mean value of the electric field as well as its variance converge against a finite value for diverging system radii and donor ionization probabilities. The resulting electric field distribution shows an $E^{-5/2}$ dependency that is well supported by the theoretical model and is additionally in good agreement with the experimentally determined spectrum of the excitonic transition.

HL 37.10 Wed 18:00 Poster F

**Characterizing broadening effects and hysteresis of donor-bound excitons in 28-Si:P** — •Dolores García de Viedma[1], 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

Our current work emphasizes how different effects affect the broadening of excitonic transitions at phosphorous donors in ultrapure isotopically enriched 28-Si. One main contribution is given by statistical electric field fluctuations due to spontaneous ionization of donors. Another point of interest is the variation of sample temperature, resulting in a shift of the bandgap [1]. Measurements are performed by LockIn-Amplification of a transmitted probe-laser signal. Linewidth data at different temperatures and varying above bandgap excitation enable the resolution of their respective influence on the line broadening for donor-bound excitons. The results are compared to numerical and analytical calculations.

[1] Sauter, et al. Phys. Rev. Research. **5**, 013182, (2023).

HL 37.11 Wed 18:00 Poster F

**Exploring locking techniques for sub-picometer-scale stabilization of open micro-cavities** — •Ayesha Khan[1,2], Jonathan Noé[1,2], Michael Förg[1,2], Manuel Nutz[1,2], Sambit Mitra[1,2], and Thomas Hümmer[1,2,3] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany — [2]Qlibri GmbH, München, Germany — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

Fiber-based, open-access micro-cavities are a new technology allowing enhancement of light-matter interactions with stability at pico-meter scale. These cavities can be used for spectroscopy of nano-scale solid state systems, single photon sources, and quantum applications such as quantum computation and quantum repeaters. Reaching ultimate stability and performing controlled sweeps is only possible by implementation of active locking techniques which are needed alongside any measurement being performed. Here, we present two different side-of-fringe locking techniques: two stop band lock and higher order mode lock. These locking techniques allow complete decoupling of the locking laser and the excitation laser. The independent excitation laser then ensures that any noise induced by active locking is not translated into the measurements. These locking techniques can be implemented in measurements of solid-sate nano-systems such as quantum dots embedded in membranes to achieve Purcell enhancement for quantum technologies and high precision spectroscopy.

HL 37.12 Wed 18:00 Poster F

**Quantum dot photon emitter for 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 Gruetzmacher[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

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. While non-linear optical processes can be used for wavelength

conversion[1], there is no well-established methods of the photon bandwidth conversion. Here, we show the design of an epitaxial quantum dot device that aim to use electrostatic gates to manipulate the bandwidth of the photons emitted from InAs quantum dots to improve the match to the spin qubits realized in ions. We show that application of electrostatic fields can change the overlap of the electron and the hole wavefunctions, leading to different radiative recombination rates. We will discuss the conditions that the heterostructure has to fulfill for the device operation and will show the status of its fabrication, which has centered on optimizing the epitaxial growth of the material. [1] A. Hamer, D. Fricker, M. Hohn, P. Atkinson, M. Lepsa, S. Linden, F. Vewinger, B. Kardynal,S. Stellmer, Opti.Lett.47,1778-1781(2022)

HL 37.13 Wed 18:00 Poster F

**Towards optical interfaces to spin qubits with epitaxial GaAs quantum dots** — •Selma Delić[1,2], Xuelin Jin[1,2], Sebastian Kindel[2], Paola Atkinson[3], Natalia Demarina[4], Hendrik Bluhm[2], Hans-Georg Babin[5], Arne Ludwig[5], Nils von den Driesch[1,6], Alexander Pawlis[1,6], Detlev Grützmacher[1,2], and Beata Kardynał[1,2] — [1]Peter Grünberg Institut (PGI) 9, Forschungszentrum (FZ) Jülich, 52428 Jülich — [2]Department of Physics, RWTH, 52074 Aachen — [3]Institut des Nano Sciences de Paris, CNRS UMR 7588, Sorbonne Université, 75005 Paris — [4]PGI 2, FZ Jülich — [5]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum — [6]PGI 10, FZ Jülich

Singlet-triplet (S-T) qubits created in gate-defined quantum dots (GDQD) at the GaAs/AlGaAs interface are promising candidates in quantum information processing. Due to the absence of hole confinement, S-T qubits cannot be directly coupled coherently to photonic qubits, which can be information carriers in quantum networks. One solution to this problem is coupling a GDQD to an epitaxial QD.

In this contribution, we show the design of heterostructures to fabricate optical interfaces to spin qubits in GaAs. We present the status of the optical and electrical characteristics of heterostructure wafers and the status of the device fabrication, focusing on the progress in spatial alignment of the two types of QDs. Using atomic force microscopy imaging, we show that the alignment can be realised by identifying and locating defects on the heterostructure's surface, which originate from the growth of GaAs QDs through local droplet etching.

HL 37.14 Wed 18:00 Poster F

**Characterisation of GaN/AlGaN-ISFET Wheatstone bridge pH-sensors** — •Alexander Hinz[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

GaN/AlGaN-heterostructure field-effect transistors as pH-sensors were investigated. A Wheatstone bridge design is used to compensate environmental drift effects due to temperature and persistent photocurrent. In that line sputtered Al2O3 is used as a passivation layer for the reference transistors. In addition, the integration of an on-chip Pt counter electrode will be discussed. Furthermore, the impact of a a GaN cap compared to an AlGaN will be analysed. The stability and the evolution of the pH sensitivity with time were investigated.

HL 37.15 Wed 18:00 Poster F

**Impact of stress current on electro-optical properties of the active cavity region in 850 nm oxide-confined vertical-cavity surface-emitting lasers (VCSEL)** — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Helmut Meinert[1], Sebastian Haberkern[1], Kevin Ehling[1], Maximilian Stock[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

VCSELs are used as efficient light sources for high-speed datacom, sensor and free-space applications. Optimization of the device performance includes an understanding of their degradation behavior under high current stress. VCSELs employing different doping of the cavity region are studied utilizing reverse current-voltage (IV) characteristics as well as photocurrent spectroscopy (PCS). Reverse IV characteristics exhibits avalanche breakdown enabling an estimation of the electric field in the cavity region. PCS reveals quantum well transitions redshifting with reverse bias due to quantum-confined Stark effect. Whereas VCSELs with a controlled doping do not show any changes VCSELs without doping of the cavity region exhibit reduced breakdown voltages being accompanied by operation-induced redshifts of quantum well transitions. These results are discussed in terms of different processes occurring during high current operation.

HL 37.16 Wed 18:00 Poster F

**High-$\beta$ lasing in photonic-defect semiconductor-dielectric hybrid microresonators with embedded InGaAs quantum dots** — •Kartik Gaur, Ching-Wen Shih, Imad Limame, Aris Koulas-Simos, Niels Heermeier, Chirag Palekar, Sarthak Tripathi, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

InGaAs quantum dots embedded in microcavities based on highly reflective distributed Bragg reflectors (DBRs) allow for the development of high Q-factor, low mode volume microcavities that feature high light-matter interaction. However, epitaxially grown DBRs consisting of GaAs/AlAs layers suffer from relatively low refractive index contrast, and often high absorption of the laser light upon optical pumping. Here, we propose an easy-to-fabricate microcavity design to produce optically pumped high-$\beta$ quantum dot microlasers. Our cavity concept is based on a buried photonic defect for tight lateral mode confinement in a quasi-planar microcavity system, which includes an upper dielectric DBR as a promising alternative to conventional III-V semiconductor DBRs. The cavities show distinct emission features with a characteristic photonic defect size-dependent mode separation and Q-factors up to 17000. Comprehensive investigations further reveal lasing operation with a systematic increase (decrease) of the $\beta$-factor (threshold pump power) with the number of mirror pairs in the upper dielectric DBR. Notably, due to the quasi-planar device geometry, the microlasers show high temperature stability.

HL 37.17 Wed 18:00 Poster F

**Optical tuning of Perylene-hybridized nanowire lasers** — •Leon Kross, Edwin Eobaldt, Jakob Wurschi, Aurelia Eberhard, Marco Grünewald, Daniel Costabel, Kalina Peneva, and Carsten Ronning — Friedrich-Schiller-Universität, Jena, Germany

Over the past decade, the exploration of the laser properties has been a focal point in semiconductor nanowire research. With the spectral and temporal characteristics well-established to date, the next step involves advancing towards their application as nano-scale coherent light sources by deliberately manipulating these properties. In this regard, the hybridization of nanowires with customized molecules might offer new knobs through efficient charge and energy transfer processes at the heterointerface. As a proof of concept, ZnO nanowires were hybridized with perylene-based dye molecules as they provide an extraordinary chemical and optical stability, and, especially, the advantage to easily tune their optical gap over a wide spectral range by chemical functionalization. In this study, we carried out comparative micro-photoluminescence measurements to examine the influence of the molecules on the nanowire lasing properties. In particular, we show how different chemical functionalization and the applied amount of dyes play a significant role for a wavelength tuning of the nanowire, which paves the way towards a highly controllable emission by tailoring the chemical structure of the dyes.

HL 37.18 Wed 18:00 Poster F

**Monolithic 850 nm VCSEL Array for QKD 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.

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 with regard to 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 an array of eight VCSELs emitting at 850 nm, capable to be used in a faint pulse source enabling QKD via the BB84 and decoy state protocol. The VCSEL structure was fabricated on a 4-inch GaAs wafer using metal-organic vapor-phase epitaxy (MOVPE), and the VCSELs are arranged in a coplanar contact design. Polarization control of the laser emission is achieved by monolithically integrated surface gratings in the light opening window of the VCSELs. Structures with surface grating reliefs were fabricated for additional modal control. The electro-optical device characteristics as well as a detailed investigation of the polar-

ization states of the VCSELs realized with the aforementioned surface gratings are presented.

HL 37.19 Wed 18:00 Poster F

**Ultrafast Femtosecond Laser Induced Dynamics of Black Silicon** — •Christelle Ines Kana Mebou[1], Tobias Zier[2], and Martin. E. Garcia[1] — [1]Institut für Physik, Universität Kassel, Germany — [2]Department of Physics, University of California Merced

Modern materials science has made manipulating material properties at the nanoscale a major focus. Due to its potential to enable novel applications in optoelectronics, photonics, and nanotechnology, the interaction of strong femtosecond laser pulses with black silicon has drawn a lot of attention. In this theoretical investigation, we investigate the dynamical and structural alterations brought about by the laser irradiation as we examine the motion of Silicon doped with Sulfur under a femtosecond laser pulse. We use a variety of methods to clarify how varied sulphur atom concentrations affect the behaviour of the material. Starting from initially randomly distributed S atoms, we simulated the ultrashort time dynamics of the system after laser heating. This research sheds light on the intricate relationship between laser-induced dynamics and dopant concentration, providing a conceptual framework that may be used to direct the development of future optoelectronic devices.

HL 37.20 Wed 18:00 Poster F

**MOVPE grown InGaAs/GaAs quantum dots as gain medium in semiconductor lasers for the telecom O-band** — •Philipp Noack, Nathalie Benzler, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart

Conventional quantum well gain media are essentially used in every commonly available laser diodes. These devices are easy to produce and are cheap in mass production. However, there are wavelength ranges, that can not be covered by quantum well gain media, due to the constraints in lattice-matched substrates and materials. Semiconductor quantum dots (QDs) as gain media are able to reach these wavelength ranges, while also providing lower threshold currents, higher temperature stability and fast gain recovery times.

To reach emission in the telecom O-band, we grow InGaAs QDs on a GaAs substrate. We achieve growth of uniform high density quantum dots in single and in up to ten vertically stacked layers by carefully controlling a variety of growth parameters, like temperature, V/III ratio and the stabilization of the surface during growth.

These quantum dot layers are incorporated into edge emitting lasers to investigate the performance as well as the temperature stability of these devices. In this way we can make sure, that vertically stacked quantum dot layers increase the modal gain without introducing defects that increase the intrinsic optical losses.

HL 37.21 Wed 18:00 Poster F

**Towards novel red-emitting VECSELs with a grating waveguide structure** — •Peter Gierss[1], Ana Ćutuk[1], Maxim Leyzner[2], Uwe Brauch[2], Marwan Abdou Ahmed[2], Michael Jetter[1], Thomas Graf[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Institut für Strahlwerkzeuge, University of Stuttgart, Pfaffenwaldring 43, 70569 Stuttgart

Classical vertical external-cavity surface-emitting lasers (VECSELs) offer favorable properties in comparison to other laser systems like e.g. near-diffraction limited beam profiles, high possible output powers and due to their external cavity, the possibility to integrate further optical elements into the cavity. Limitations arise due to the incorporation of a thick distributed Bragg reflector (DBR), which restricts the available laser wavelength and also possesses poor thermal properties.

A new design for a VECSEL is based on the use of a grating-waveguide structure (GWS) over the active region. In combination with a low-refractive-index heat spreader, the leaky guided-mode resonances of the GWS lead to a broadband high reflectivity of the device, which is required for efficient laser operation.

In this contribution we present our recent progress in the development and fabrication of this device.

HL 37.22 Wed 18:00 Poster F

**In-plane coupling between a WGM micro-ring and a ridge waveguide** — •Léo J. Roche[1], Yuhui Yang[1], Fridtjof Betz[2], Ching-Wen Shih[1], Aris Koulas-Simos[1], Sven Burger[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik (TUB), Berlin, Germany — [2]Zuse Institute Berlin, Berlin, Germany

Integrated quantum photonic circuits (IQPCs) are very promising candidates for scalable and flexible on-chip quantum computation and quantum communication hardware. One critical requirement for their realization is the scalable integration of on-demand indistinguishable single-photon emitters. This is potentially possible through the resonant excitation of an integrated QD in a waveguide by means of an on-chip integrated coherent light microlaser. Towards this goal, we investigate the coupling and lasing properties of coherent light laterally emitted from a whispering gallery mode (WGM) type micro-ring resonator evanescently coupled to a single mode ridge waveguide. Using finite element method (FEM) simulations, we investigate the optimal geometrical parameters maximising the coupling efficiency between the two structures. The III-V semiconductor type nanostructures composed of a GaAs cavity with InGaAs QDs, on top of a SiO2 layer are processed using high-resolution electron beam lithography. Various geometries of the micro-ring coupled to waveguide with grating outcoupler are processed and subsequently investigated via micro-photoluminescence spectroscopy to provide a systematic study.

HL 37.23 Wed 18:00 Poster F

**Optically pumped micropillar lasers at room temperature for gas sensing around 960 nm** — •Floriana Laudani, Sarthak Tripathi, Kartik Gaur, Aris Koulas-Simos, Sven Rodt, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany

Quantitative water vapor measurements are essential for industrial applications to ensure a qualitative processing and control chain and require gas sensors with short response times and narrow spectral bandwith in a broad wavelength range. In contrast to conventional edge-emitting lasers, compact surface-emitting lasers offer a cost-effective alternative, usable in a variety of gas-sensing systems, with respect to the emission wavelength.

We report on room temperature operation of optically pumped GaAs micropillar lasers with a set of $In_{0.33}Ga_{0.67}As$ quantum dot (QDs) layers as active gain medium embedded in an $Al_{0.2}Ga_{0.8}As/Al_{0.9}Ga_{0.1}As$ distributed Bragg reflector (DBR) microcavity structure, emitting at a target wavelength of around 960 nm. The fabrication process is based on high-resolution electron-beam lithography with subsequent suitable development steps. The micropillars are made by etching in an Inductively Coupled Plasma RIE (ICP-RIE) chamber using a $CL_2/BCL_3/Ar$ atmosphere.

HL 37.24 Wed 18:00 Poster F

**Electrical and Magnetotransport of the correlated metal $CaVO_3$** — •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 Berlin, 12489 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 of the Science of Materials Berlin, 12489 Berlin, Germany

High-performance and cost-effective transparent conductive materials are in great demand in the optoelectronic industry. Correlated metals offer an alternative strategy to design a material with both high-optical transparency and high-electrical conductivity. In order to test this, the transport phenomena in these materials must be studied [1].

We have recently studied the electric transport characteristics of thin $CaVO_3$ films, which exceeded a residual-resistivity ratio *RRR* of 90 [2]. In this work, we study the temperature-dependent resistivity, Hall- and magneto-resistance between 4.2 K and 300 K. Films with high *RRR* showed increasingly nonlinear Hall resistivities and linear magnetoresistance below 40 K. Deviations from the Fermi liquid $T^2$ dependence of the resistivity were also observed. These deviations are discussed together with a multi-carrier model and the influence of the complex Fermi surface of $CaVO_3$ on the transport properties.

[1] Zhang, Lei, *et al.*; Nature materials **15.2**, 204-210 (2016).
[2] Tatiana Kuznetsova, *et al.*; APL Mater. ; **11 (4)**: 041120 (2023).

HL 37.25 Wed 18:00 Poster F

**Electronic band structure and thermoelectric properties of ternary SnSxSe2-x (x = 0,1,2)** — Aliakbar Ghafari[1,2] and •Christoph Janowitz[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Department of Inorganic Chemistry, Fritz-Haber-Institut

der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [3]Humboldt Universität, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

We present a theoretical investigation of the electronic structure of layered metal dichalcogenides ternary SnSxSe2-x, with x = 0, 1, and 2. (A. Ghafari, C. Janowitz, Materialstoday Comm. 38, 107483, (2024)). Calculations involved density functional theory (DFT), density functional perturbation theory (DFPT), and Boltzmann transport theory. It has been found that adding Sulfur to the structure leads to an increase in i) direct and indirect band gaps, ii) the Seebeck coefficient iii) the acoustic and optical branches iv) the power factor and v) the lattice thermal conductivity. The thermoelectric properties are studied from the first principle for the whole series of compositions at the highest achievable n- and p-doping levels.

HL 37.26 Wed 18:00 Poster F

**Tuning the optical properties and transient dynamics of antimony through external fields** — •Joel Billermann, Sebastian Walfort, Niklas Vollmar, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

The crystal structure of antimony is characterized by a Peierls distortion motif resulting from a subtle energy balance between the electronic and atomic subsystems [1]. Perturbing this energy balance through the impulsive excitation of a small fraction of valence electrons leads to large structural changes towards a more symmetric phase and the displacive excitation of coherent phonons [2]. The system then decays back to the distorted structure within picoseconds. In our present study, we explore schemes to permanently shift the potential energy landscape of antimony towards the symmetric phase by applying external electric and strain fields. We use steady-state- and femtosecond pump-probe spectroscopy to elucidate the influence of structural distortion on both the optical properties and the ultrafast photoinduced dynamics of antimony, e.g. the coupling of the electron system to the lattice.

[1] U. Argaman et al., J Phys Condens Matter 31, 465501 (2019)
[2] H. J. Zeiger et al., Phys. Rev. B 45, 768 (1992)

HL 37.27 Wed 18:00 Poster F

**Tailored sample designs for ultrafast electron diffraction at high repetition rates** — •Leonardo C. da Camara Silva[1,2], Till Domroese[1,2], and Claus Ropers[1,2] — [1]4th Physical Institute, University of Göttingen, Germany — [2]Max Planck Institute for Multidiscipinary Sciences, Göttingen, Germany

Ultrafast electron diffraction (UED) is a powerful technique to resolve structural dynamics in strongly-correlated materials on ultrafast timescales [1]. For these experiments, the high-coherence electron source of the Göttingen Ultrafast Transmission Electron Microscope (UTEM) [2] enables the formation of particularly narrow but highly collimated femtosecond electron pulses. The nanometric beam diameters give access to nanoscale heterogeneity that often decisively influences the dynamics [3]. Highest spatiotemporal resolution, however, is only achieved for low bunch charges, mitigating Coulomb-induced pulse broadening, such that diffraction signal critically depends on the available duty cycle of the experiment. Here, we characterize different sample designs tailored to confine the laser excitation volume and to efficiently dissipate the thermal load. This allows us to drastically enhance the available repetition rates in our UED measurements, investigating structural phase transitions in the charge-density wave material 1$T$-$TaTe_2$ at rates up to 2 MHz.

[1] D. Filippetto et al., Rev. Mod. Phys. **94**, 045004 (2022)
[2] A. Feist et al., Ultramicroscopy **176**, 63-73 (2017)
[3] T. Domröse et al., Nat. Mater. **22**, 1345-1351 (2023)

HL 37.28 Wed 18:00 Poster F

**Probing the ultrafast dynamics of photonic devices based on phase change materials** — •Nils Weber, Sebastian Walfort, Niklas Vollmar, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

Phase change materials (PCMs) are compounds typically composed of germanium, tellurium and antimony. They are characterized by a strong contrast in electrical and optical properties between crystalline and glassy states. Combined with the ability to switch rapidly between crystal and glass, this contrast makes them an interesting material system for non-volatile memory elements in electronic and photonic circuits. By using photons instead of electrons as signal carriers, photonic circuits are free from the bandwidth constraints associated with electrical circuits and are therefore sensitive to material dynamics on picosecond timescales. The implications and potential new applications of operating the PCM-based memory elements at these bandwidths remain largely unexplored. Here we present the design and implementation of an experimental setup capable of resolving the ultrafast response of photonic devices. Our approach combines an amplified femtosecond free-space laser with fiber coupled ultrafast light sources in a setup with sufficient spatial resolution to address individual microscopic devices. We show first experimental results together with finite element simulations of the transient response of PCM-based optical weights as used in photonic integrated circuits for in-memory computing.

HL 37.29 Wed 18:00 Poster F

**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 38: Oxide Semiconductors II

Time: Thursday 9:30–11:30 Location: ER 325

HL 38.1 Thu 9:30 ER 325

**Energy and thickness dependent intensity characteristics of simultaneous XEOL-XAS measurements of ZnO** — Sergiu Levcenko[1], Konrad Ritter[1], Hans H. Falk[1], Timo Pfeiffelmann[1], Lukas Trefflich[1], Edmund Welter[2], 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

X-ray excited optical luminescence (XEOL) is used to study optically active centers in a variety of materials. Combined with spatial and temporal resolution, XEOL is applied for multimodal analysis of hetero- and nanostructures while simultaneous XEOL and X-ray absorption spectroscopy (XAS) experiments can provide element and site selective structural information. However, no comprehensive model for the X-ray fluorescence (XRF) and XEOL intensities has yet been established. Therefore, we performed a systemtatic XEOL-XAS study of ZnO with 1 to 500 $\mu$m thicknesses at beamline P65 of PETRA III. The XRF and XEOL near-band-edge (NBE) intensities show a positive edge jump when scanning across the Zn K-edge for all samples. In contrast, the XEOL defect signal exhibits a positive edge jump for thin samples but an inverted intensity profile for thick samples. We demonstrate that all energy and thickness dependent intensity features for XRF, XEOL NBE and XEOL defect signals can be reproduced by a generalized model if the (i) experimental geometry, (ii) creation of excitations, (iii) diffusion and recombination of generated carriers and (iv) re-absorption of XRF and XEOL photons are taken into account.

HL 38.2 Thu 9:45 ER 325

**Simulation of multi-component target ablation: a novel combinatorial pulsed laser deposition technique** — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics

Combinatorial pulsed laser deposition (C-PLD) has become a well-established method in combinatorial material science. With radial and azimuthal target segmentation discrete material libraries with samples of homogeneous composition as well as samples with a continuous composition spread can be obtained from a single target. Thus, target and substrate consumption is significantly reduced. However, powder blending, insufficient hardening or thermic decomposition due to deviating sintering temperatures of the source powders for the respective target segments make the fabrication of such targets technically demanding.

In this work we present two novel deposition approaches for C-PLD which bypass the above mentioned challenges of target preparation. Both techniques allow discrete material libraries covering the entire binary phase diagram. Experimentally, $n$-type semiconducting zinc-tin-oxide thin films were fabricated with the novel C-PLD approaches, and elemental distributions are well described by simulations made beforehand. Electrical properties are compared to such of zinc-tin-oxide thin films prepared by conventional PLD.

HL 38.3 Thu 10:00 ER 325

**Molecular beam epitaxy of $\varepsilon/\kappa$-$Ga_2O_3$ using In as a surfactant** — •Alexander Karg, Alexander Hinz, Marco Schowalter, Niklas Krantz, Patrick Vogt, Stephan Figge, Andreas Rosenauer, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Bremen, Germany

This study is focused on the metastable orthorhombic $\varepsilon$-$Ga_2O_3$, for which a high spontaneous polarization along the c-axis is predicted, thus making two-dimensional electron gases with high sheet carrier densities at heterointerfaces conceivable [1]. The initiation of the $\varepsilon$-$Ga_2O_3$ growth by MBE requires the use of additives like Sn, added under Ga metal-rich growth conditions [2].

We present a systematic investigation of the role of In as a surfactant for MBE-growth of $\varepsilon$-$Ga_2O_3$ [3]. Starting from an $\varepsilon$-$Ga_2O_3$ buffer layer, realized by initial deposition of an ultrathin $SnO_2$ layer on the c-$Al_2O_3$ substrate[4], we deposited $\varepsilon$-$(In,Ga)_2O_3$ layers with varied In flux. The structural properties, the surface morphology and the In concentration in the resulting $\varepsilon$-$(In,Ga)_2O_3$ layers were investigated by X-ray diffraction, atomic force microscopy and scanning transmission electron microscopy. Based on these results we discuss the role of In as a surfactant during growth of $\varepsilon$-$Ga_2O_3$. Additionally, we demonstrate the use of indium as a surfactant to realize $\varepsilon$-$(In,Al,Ga)_2O_3$ heterostructures with well-defined and sharp interfaces.

[1] Macchioni et al., Appl. Phys. Exp. 9, 041102 (2016). [2] Kracht et al., Phys. Rev. Appl. 8, 054002 (2017). [3] Karg et al., APL Mater. 11, 091114 (2023). [4] Karg et al., J. Appl. Phys. 132, 195304 (2022).

HL 38.4 Thu 10:15 ER 325

**Ultrawide Bandgap Semiconductor Cubic Spinel $Zn_2GeO_4$ Epitaxial Thin Films** — •Jingjing Yu, Sijun Luo, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth System Sciences, Universität Leipzig, 04103 Leipzig

It is significant to explore new ultrawide bandgap oxides thin films with a bandgap larger than 4 eV for potential applications in power electronics and deep-UV photodetectors. Cubic spinel $Zn_2GeO_4$ is a high-temperature and high-pressure metastable phase, to date, only the synthesis and crystal structure are reported. In this work, we report the heteroepitaxial growth of (100)-oriented cubic spinel $Zn_2GeO_4$ thin films on cubic spinel (100) $MgAl_2O_4$ single crystal substrates using pulsed laser deposition. The 350 nm thick (100) $Zn_2GeO_4$ epitaxial thin film shows a full width at half maximum of rocking curve of (800) reflex of about 0.35°. The direct optical bandgap is evaluated to be about 5 eV. The resistivity of film decreases gradually from about 4.0 to 0.5 Ω cm as temperature increases from 50 to 350 K. The Hall electron carrier mobility increases from 4.3 to 28.4 $cm^2\ V^{-1}s^{-1}$ while the Hall electron carrier concentration slightly increases from about 3.5 x $10^{17}$ to about 4.6 x $10^{17}$ $cm^{-3}$ as the temperature increases from 50 to 350 K. The n-type conductivity probably originates from oxygen vacancies-related defects, as the post annealing at high temperatures in the air could make the thin film become insulating. This work advances the fundamental research on ultrawide bandgap cubic spinel $Zn_2GeO_4$ semiconductor thin films for potential device application.

**15 min. break**

HL 38.5 Thu 10:45 ER 325

**Growth, faceting and thickness effects of $\alpha$-$Ga_2O_3$ and $\alpha$-$(In_xGa_{1-x})_2O_3$ on $m$-plane $\alpha$-$Al_2O_3$ by molecular beam epitaxy** — •Martin S. Williams[1], Manuel Alonso-Orts[1], Marco Schowalter[1], Alexander Karg[1], Sushma Raghuvansy[1], Jon P. McCandless[2], Debdeep Jena[2], Andreas Rosenauer[1], Martin Eickhoff[1], and Patrick Vogt[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, Bremen, 28359, Germany — [2]School of Electrical and Computer Engineering, Cornell University, 229 Phillip's Hall, 14853, New York, United States of America

Gallium oxide ($Ga_2O_3$) is a promising ultra-wide band gap semiconductor, especially for high-power electronics which are crucial for reducing loss in power converters [1]. The corundum-structured phase ($\alpha$-$Ga_2O_3$) has seen particular interest – owing to its large band gap, of 5.3 eV [2]. Its isostructurality to $\alpha$-$Al_2O_3$ allows for band gap engineering of $\alpha$-$(Al_xGa_{1-x})_2O_3$ over the entire Al compositional range [2]. Achieving single-crystalline $\alpha$-$Ga_2O_3$ thin films is therefore important for developing future $\alpha$-$Ga_2O_3$-based devices.

In this work, conventional plasma-assisted molecular beam epitaxy (MBE) and metal-oxide-catalysed epitaxy (MOCATAXY) have been employed to grow $\alpha$-$Ga_2O_3(10\bar{1}0)$/$\alpha$-$Al_2O_3(10\bar{1}0)$. By varying the O-to-Ga and In-to-Ga flux ratios, a systematic approach was taken to characterise the films and develop a growth diagram.

[1] C. V. Prasad and Z.S. Rim, Materials Today Physics 27 (2022).
[2] R. Jinno et al., Science Advances 7 (2021).

HL 38.6 Thu 11:00 ER 325

**Analysis and prediction of thickness distributions for combinatorial pulsed laser deposition** — •Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, 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. Our combinatorial pulsed laser deposition (c-PLD) method allows for the deposition of entire material libraries on e.g. a single substrate [1]. Accompanied

by the usage of high-throughput measurements such as spectroscopic ellipsometry and X-ray diffraction, the characterization of the material systems' physical properties with high chemical resolution and comparably low efforts becomes feasible [2]. By employing the plasma plume expansion model suggested by Anisimov *et al.* [3] and the resulting spatial material-deposition distribution we calculate binary growth rates as function of position on the substrate enabling us to predict film thickness and composition. As a case in point, the deposition of sesquioxide materials can be described exceptionally well over a large range of PLD parameters. Using these results we demonstrate that the binary distributions can be used to predict the thickness- and compositional distributions for ternary alloys grown with c-PLD with high precision. [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 38.7 Thu 11:15 ER 325

**Phase-selective growth of $\kappa$- vs $\beta$-$Ga_2O_3$ and $(In_xGa_{1-x})_2O_3$ by In-mediated metal exchange catalysis in plasma-assisted molecular beam epitaxy** — •Andrea Ardenghi[1], Oliver Bierwagen[1], Jonas Lähnemann[1], Joe Kler[2], Andreas Falkenstein[2], Manfred Martin[2], and Piero Mazzolini[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Institute of Physical Chemistry, RWTH Aachen University, D-52056 Aachen, Germany — [3]Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delle Scienze 7/A, 43124 Parma, Italy

Monoclinic $\beta$-$Ga_2O_3$ is an ultra-wide bandgap semiconductor (Eg $\approx$ 4.8 eV) that is attracting increasingly attention for power electronics applications. The metastable kappa polymorph ($\kappa$-$Ga_2O_3$), which shares a comparable bandgap, exhibits piezoelectric and potentially ferroelectric properties. In-incorporation into any polymorphs of $Ga_2O_3$ allows to lower their bandgap. In this work, we provide a guideline to achieve single phase $\kappa$-, $\beta$-$Ga_2O_3$ as well as their $(In_xGa_{1-x})_2O_3$ alloys up to x = 0.14 and x = 0.17 respectively, using In-mediated metal exchange catalysis in plasma assisted molecular beam epitaxy (MEXCAT-MBE). The polymorph transition from $\kappa$ to $\beta$ is addressed, highlighting the role played by the thermal stability of the $\kappa$-$Ga_2O_3$. Additionally, we demonstrate the growth of (-201) $\beta$-$Ga_2O_3$ on c-$Al_2O_3$ at temperatures at least 100 °C above those achievable with conventional non-catalyzed MBE.

## HL 39: Outreach / Wissenschaftskommunikation

Organized by Axel Lorke.

Time: Thursday 9:30–10:45 Location: EW 015

HL 39.1 Thu 9:30 EW 015

**Curiosity through a playful approach** — •Gérald Kämmerer — Faculty of Physics, University of Duisburg-Essen

No one is more enthusiastic than children and teenagers. After all, they're the physicists of tomorrow, right? As soon as they start physics classes at school, many children and teenagers lose interest in physics and everyday phenomena. For them, physics is often a dry, inaccessible set of formulas and facts. But it is precisely with children and teenagers that one can work with curiosity and enthusiasm. That is why I give talks at events like "freestyle-physics" or the "Lange Nacht der Physik" at the University of Duisburg-Essen. In my talk, I show how I manage to inspire children, teenagers and even teachers again and again. Here, I want to show how I use a playful approach to teach physics in reality and everyday phenomena.

HL 39.2 Thu 9:45 EW 015

**ScienceQorner: Wissenschaft im Radio** — •Laura Nicolette Schusser — Physikalisches Institute der Universität Münster, Münster, Germany — Radio Q, Münster, Germany

Radio Q ist das Campusradio für Münster und Steinfurt. Das Programm wird durch ehrenamtliche Studierende von den verschiedenen Hochschulen in Münster gestaltet. Dabei ist das Ziel von Radio Q Programm von Studierenden für Studierenden zu machen. Außerdem soll Radio Q Studierenden eine Plattform bieten, das Radiohandwerk zu erlernen und neue Dinge auszuprobieren. In diversen Formaten berichten wir unter anderem über neuste wissenschaftliche Erkenntnisse, aus der Physik und darüber hinaus. Wie Wissenschaftsvermittlung in einem Campusradio funktioniert und wo die Unterschiede zu großen Medienhäusern liegen, wird in dieser Session besprochen.

HL 39.3 Thu 10:00 EW 015

**More than just Big Bang Theory – Demystifying particle acceleration facilities for the public** — •Lea Kämmerer, Gérald Kämmerer, and Tobias Lojewski — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), Univeritsy of Duisburg-Essen, 47057 Duisburg, Germany

When talking with people about my job as an experimental physicist, they often have different associations with characters from popular culture. One such example is Leonard from the show The Big Bang Theory. Others are discouraged by the term "physics" and claim that it is too complicated. Physics is more than just what we see on TV. There are many exciting concepts that anyone can understand if they are communicated in the right way. That's why I've started making short videos for the SFB1242. In these clips, I show what happens at large particle acceleration facilities, like a synchrotron, and take people by the hand and walk them through these fascinating workspaces. In my talk, I want to show you how we managed to record these videos as a team during the beamtimes, thus allowing the public to participate in this fascinating field of physics.

HL 39.4 Thu 10:15 EW 015

**Developing a structured training and further education program in quantum technologies - an overview of the Quantum LifeLong Learning course program** — •Judith Gabel[1], Björn Ladewig[1], Christos Paspalides[2], Anna Donhauser[1], Stefan Küchemann[1], Jochen Kuhn[1], Tatjana Wilk[1], Alexander Holleitner[2], and Jan von Delft[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Technische Universität München, Germany

Quantum technologies have the potential to disrupt various industries. As these technologies mature and transition from university research labs to real-world industry applications, it thus becomes increasingly important for professionals across different disciplines to acquire a comprehensive understanding of their capabilities and applications. Acknowledging this need, the Quantum LifeLong Learning (QL3) project, an initiative from the Munich universities, has been established. The QL3 project is a training and further education program tailored for diverse target groups within the industry. It caters to professionals ranging from managers and leaders without a technical background who seek an overview of quantum technologies over engineers looking for a thorough understanding of the field to quantum experts seeking a detailed introduction to fault-tolerant quantum computing. We outline our course program and share insights from the lessons we learned during its development.

HL 39.5 Thu 10:30 EW 015

**Live Stratosphären MINT Projekt** — •Volker Tympel[1,2], Immo Kadner[3] und Bernd Schirmer[3] — [1]Helmholtz-Institut Jena, Jena — [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt — [3]NaWi School Verein Naturwissenschaftliche Bildung e.V., Panketal

Kiste packen, Ballon starten, Bergung, mit etwas Glück am nächsten Tag die Datenauswertung, das ist der Ablauf für eine Schulhof Forschungsmission in die Stratosphäre. Ballon starten, live Verfolgung und Datenerfassung in Klassenzimmer oder Aula, das geht - wie hier beschrieben wird - mit Amateurfunkunterstützung und entsprechender Hard- und Software. Am Beispiel eines speziellen Geiger-Müller Zählers (GMC) wird gezeigt, wie die Messwerte zum Regener-Pfotzer Maximum der sek. kosm. Strahlung direkt auf einen Beamer kommen. Die gezählten Ereignisse steigen dabei von ca. 25 cpm auf ca. 600 in etwa 20 km Höhe, um dann wieder abzunehmen. Die Datenübertragung erfolgt über das XDATA Protokoll, welches auch bei kommerziellen Radiowettersonden für zusätzliche wissenschaftliche Instrumente

benutzt wird. Die aktuelle RS41Tracker Dekodier-Software kann die Mess- und Betriebswerten darstellen. Bis zu 6 Instrumenten können an einen Sender gekoppelt werden. Darüber hinaus ist es auch möglich, den GMC selbst auf zu bauen. Es gibt einen Löt-Bausatz mit Leiterplatte, allen notwendigen Bauteilen und einem Gehäuse. Basis ist ein Arduino-Nano. Es braucht aber einige Tage, etwas Messtechnik und fachliche Anleitung, um die 13 Einzelschritte mit den entsprechenden Tests zu absolvieren.

## HL 40: 2D Materials and Heterostructures: Magnetic Properties

Time: Thursday 9:30–13:00 Location: EW 201

HL 40.1 Thu 9:30 EW 201

**Optical properties of quasi-one-dimensional materials** — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Many of the atomically thin materials used today, such as graphene or $MoS_2$, exhibit a high in-plane symmetry. Anisotropic crystals unite the fascinating characteristics of the confined in-plane physics with their reduced crystal symmetry. This paves the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.

Here, we investigate and compare the doping-dependent optical properties of three different classes of materials from a first-principles perspective. Besides the well-known black phosphorus and the transition metal dichalcogenides $ReS_2$ and $ReSe_2$, we study the in-plane ferromagnetic CrSBr. Although all materials have a distinct anisotropy, the influence on the optical properties is intimately linked to the nature of the electronic quantum states.

HL 40.2 Thu 9:45 EW 201

**Magnetic anisotropy in excitonic resonances and exciton-phonon coupling of the 2D magnetic semiconductor CrSBr** — •Pierre-Maurice Piel[1], Nicolai-Leonid Bathen[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

The van der Waals material CrSBr comprises several intriguing characteristics: it is an optically active semiconductor and an air-stable 2D magnet with ferromagnetic ordering within each layer and antiferromagnetic coupling between adjacent layers. It has also a highly anisotropic electronic band structure, rendering it a quasi-one-dimensional electronic system [1]. In order to unravel the impact of magnetic order and magnetization direction on various aspects, including excitonic interband transitions, exciton-phonon coupling, and collective excitations, we employ magnetic field-dependent photoluminescence and resonant Raman experiments at low temperatures, around 4 Kelvin, well below the Néel temperature. We observe distinct differences for anti-ferromagnetic and ferromagnetic order in in the excitonic signatures from PL measurements and in resonant Raman spectra, both showing magnetic anisotropy for different crystallographic orientations. While the Raman-allowed first order phonon modes are unaffected by magnetization direction, new and well resolved magnetic-field dependent modes occur in the resonant-Raman spectra indicating strong exciton-phonon coupling. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023)

HL 40.3 Thu 10:00 EW 201

**Proximity effects in the valley Zeeman physics of van der Waals heterostructures** — •Paulo E. Faria Junior and Jaroslav Fabian — University of Regensburg

Proximity effects are a hallmark of van der Waals systems, providing a very efficient way to functionalize the different materials in the heterostructure. Interestingly, these proximity effects arise from the small overlap of electron densities within the van der Waals gap. In this talk, I will address how proximity effects can be observed using the valley Zeeman physics of excitons in van der Waals heterostructures. Specifically, I will focus on three different scenarios: (i) the impact of electric field and interlayer distance fluctuations to interlayer exciton g-factors in MoSe2/WSe2 heterostructures[1]; (ii) the unexpected proximity-enhanced valley Zeeman shift in WS2/graphene systems[2]; and (iii) the emergence of an asymmetric valley Zeeman shift in MoSe2/CrSBr structures[3]. [1] Faria Junior, Fabian, Nanomaterials 13, 1187 (2023). [2] Faria Junior et al., 2D Mater. 10, 03400 (2023). [3] Serati de Brito, Faria Junior et al., arXiv:2309.03766, to appear in Nano Letters (2023). Funding: DFG SFB 1277.

HL 40.4 Thu 10:15 EW 201

**Computational design of two-dimensional cold metal lateral heterojunction (Nb/Hf)$Si_2N_4$ tunnel diodes** — •Paul Bodewei, Ersoy Sasioglu, Nicki Frank Hinsche, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany

Cold metals have recently gained attention as a promising platform for innovative devices, such as tunnel diodes with negative differential resistance (NDR) [1] and field-effect transistors with subthreshold swings below the thermionic limit. Recently discovered two-dimensional (2D) transition metal carbides and nitrides have both metallic and semiconducting properties, making them ideal for these applications. We present a computational study of a prototype $NbSi_2N_4/HfSi_2N_4/NbSi_2N_4$ lateral heterojunction tunnel diode. Using density functional theory and a nonequilibrium Green function method, we investigate the current-voltage characteristics of these diodes with varying barrier thicknesses in zigzag and armchair orientations. Our results indicate negative differential resistance that leads to unconventionally high peak-to-valley current ratio (PVCR). Moreover, significant differences in peak current densities as well as PVCR for both armchair- and zigzag-orientations of the tunnel diodes have been found. These findings suggest that cold metal based materials hold promise for high PVCR NDR tunnel diodes, with potential applications in memory, logic circuits, and electronic devices. [1] Ersoy Şaşıoğlu and Ingrid Mertig, ACS Appl. Nano Mater. 6, 3758-3766 (2023).

HL 40.5 Thu 10:30 EW 201

**Optical signatures of the magnetic order in 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

Controlling excitons in van der Waals coupled systems is a key idea to reveal tailored properties for the development of opto-electronic devices. Exciton energy and character in antiferromagnetic multilayer CrSBr can be controlled by an external magnetic field switching the internal magnetization to a ferromagnetic order. This modifies the optical response and we observe in our ab-initio GW/BSE calculations a distinct redshift, in accordance with corresponding measurements. We set up a minimal model to explain and convey the underlying physical mechanisms. Depending on the external field the coupling of adjacent layers is changed, shifting electronic states linearly in energy and excitons quadratically with respect to the field strength. While our results are generally valid for antiferromagnetic layered magnets, we uncover that the lowest excitation in CrSBr is optically dark and its detuning can also be controlled by the magnetic field.

HL 40.6 Thu 10:45 EW 201

**Spectral-imaging of 2D magnetic semiconductor V-WS2 using ToF-XPEEM** — •Q. Nguyen[1], O. Tkach[2,3], O. Fedchenko[2], S. Chernov[4], Z. Zhang[5], L. Hoang[5], M. Prandolini[4], D. Kutnyakhov[4], F. Pressacco[4], J. Dilling[4,7], L. Bruckmeier[4,7], M. Scholz[4], F. Scholz[4], C. Schlueter[4], K. Rossnagel[4,7], M. Kling[1,5], M. Hoesch[4], E. Pop[5], A. Mannix[5], T. Gorkhover[4,8], M. Dunne[1,5], N. Sirica[6], R. Schoenlein[1], H.-J. Elmers[2], and G. Schoenhense[2] — [1]SLAC Nat. Accel. Lab., USA — [2]Univ. Mainz — [3]SumDU, Ukraine — [4]DESY — [5]Stanford Univ., USA — [6]Los Ala. Nat. Lab., USA — [7]CAU Kiel — [8]Univ. Hamburg

Using x-ray element-selective, time-of-flight photoemission electron microscopy (ToF-XPEEM), we characterize the spatial distribution and spectroscopic signatures of p-type vanadium dopant within the 2D semiconductor WS2 - achieving unprecedented 1.0-micron spatial resolution. Multilayer WS2 islands ranging from 3 - 20-micron in lat-

eral size are grown via hybrid metal-organic chemical vapor deposition with nominal vanadium dopant concentrations ranging from 4 to 30 atom%. Combined with the soft x-ray energies at PETRA III - P04, ToF-XPEEM measurements reveal unique elemental spectroscopic signatures that reflect the stoichiometry within each island - which is important for optimizing the growth of these semiconductors. The spatial maps unravel the atomic positions of vanadium and tungsten within the 2D flakes at different doping concentration. Complementary full-field, hard x-ray photoelectron diffraction measured at PETRA III - P22 and Bloch wave calculations reveal the structural properties.

**15 min. break**

**Invited Talk** HL 40.7 Thu 11:15 EW 201

**Exciton transport in van der Waals antiferromagnet CrSBr** — •Florian Dirnberger[1], Sophia Terres[1], Akashdeep Kamra[2], Mikhail M. Glazov[3], and Alexey Chernikov[1] — [1]Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Saint Petersburg, Russia

The recent discovery of magnetic excitons - a rare type of optical excitation that emerges from spin-polarized electronic states in magnetic materials - raises important questions about elemental interactions between excitons, magnons, and light. Particularly the prototypical layered antiferromagnetic semiconductor CrSBr and its strongly bound excitons with large oscillator strength offer exceptional opportunities in this regard. In this talk, I will present the results of our study of the spatial transport of excitons in CrSBr with particular focus on the specific role of crystal anisotropy, magnons and magnetic order. Our experiments demonstrate highly non-linear exciton transport with unusual temperature dependence that culminates in substantially enhanced exciton propagation at the antiferromagnet-to-paramagnet phase transition. Observations of anomalous and effectively negative transport further highlight the profound coupling of excitonic, vibronic, and magnetic degrees of freedom in CrSBr.

HL 40.8 Thu 11:45 EW 201

**Optoelectronic investigation of Berry curvature dipole induced non-linear anomalous thermal Hall effect in type-II Weyl Semimetal $WTe_2$** — •Ernst Knöckl[1,2] and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Munich, Germany — [2]TU Munich, Germany

The Berry curvature forms the foundation for the topological classification of band structures. Importantly, it also impacts a material's (opto-)electronic properties, for example by introducing an anomalous transversal correction to the group velocity of charge carriers. Generally, symmetry constraints often preclude the observation of such effects, and only few, low-symmetry materials directly show relevant topological transport properties. In particular, few-layer $WTe_2$ has been shown to exhibit a nonlinear anomalous Hall effect [1] due to its low crystal symmetry and its strong Berry curvature dipole (BCD). We discuss the requirements for optically detecting a so far elusive thermal analogue of this effect, which is the socalled nonlinear anomalous thermal Hall effect (NLATHE). In principle, the NLATHE allows for experimentally accessing the first derivative of the BCD with respect to the chemical potential [2]. We present first results obtained on few-layer $WTe_2$ integrated into on-chip thermal circuits made from silicon nitride membranes.

[1] Sodemann, I., *et al.* Physical Review Letters 115.21 (2015): 216806
[2] Zeng, C., *et al.* Physical Review Research 2.3 (2020): 032066

HL 40.9 Thu 12:00 EW 201

**Proximity Spin Physics in Twisted van der Waals Heterostructures** — •Klaus Zollner[1], Paulo E. Faria-Junior[1], Simão M. João[2], Branislav K. Nikolić[3], and Jaroslav Fabian[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Imperial College London, London SW7 2AZ, United Kingdom — [3]University of Delaware, Newark, DE 19716, USA

A crucial degree of freedom, to tailor proximity-induced spin interactions in van der Waals heterostructures, is the relative twist angle between the monolayers. We present comprehensive DFT-based results on twist- and gate-tunable proximity spin-orbit and exchange coupling in various 2D material heterostructures. Remarkably, in graphene/$Cr_2Ge_2Te_6$, the proximity exchange splitting of Dirac states can be reversed upon twisting, from 4 to −4 meV, while keeping the magnetization of $Cr_2Ge_2Te_6$ fixed [1]. In $WSe_2/CrI_3$, the valley splitting shows a gigantic tunability, from 0 to 12 meV (≈ 60 Tesla), combining twisting and gating [2]. In graphene/transition-metal-dichalcogenide bilayers, the spin-orbit coupling of proximitized Dirac bands can be tailored by several means [3]. Finally, we demonstrate the emergence of purely radial spin-orbit fields in twisted multilayers. We also relate our findings to experimentally verifiable fingerprints of proximity-induced spin interactions.

We acknowledge funding through DFG SFB 1277, DFG SPP 2244, and EU Horizon 2020 Program (Graphene Flagship).

[1] K. Zollner et al., PRL 128, 106401 (2022). [2] K. Zollner et al., PRB 107, 035112 (2023). [3] K. Zollner et al., arXiv:2310.17907 (2023).

HL 40.10 Thu 12:15 EW 201

**Impact of proximity exchange coupled $CrI_3$ on $WSe_2$ valley dynamics** — •Marc Schütte[1], Jo Bertram[1], Frank Volmer[2], Kenji Watanabe[3], Takashi Taniguchi[4], Christoph Stampfer[1], Lutz Waldecker[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics A and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]AMO GmbH, Advanced Microelectronic Center Aachen (AMICA), Aachen, Germany — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

The optical selection rules of the transition metal dichalcogenides allow to individually address and manipulate their two energetically degenerate, but distinct, valleys in k-space. Lifting the degeneracy of the valley degree of freedom is possible via magnetic proximity coupling of adjacent layered magnetic materials. Here, thin layers of the two-dimensional layer-antiferromagnet $CrI_3$ are put into direct contact with monolayer $WSe_2$.
We present our findings about the valley dynamics in electrostatically gated, proximity exchange coupled $CrI_3/WSe_2$ heterostructures by optical reflection spectroscopy and time-resolved Kerr measurements. In particular, we find a type-II band alignment. This leads to charge separation within the heterostructure and long-lived valley polarizations within the $WSe_2$ valence bands. Excited polarizations furthermore show helicity dependent lifetime differences at particular gate voltages, which emerge from the modified band structure at K and K′.

HL 40.11 Thu 12:30 EW 201

**Magnetic Field Dependent Raman Scattering in 2D Materials and Thin Films** — •Hans Tornatzy, Manfred Ramsteiner, Joao Marcelo J. Lopes, and Markus R. Wagner — Paul-Drude-Institut, Berlin

Raman scattering by optical phonons in nonmagnetic materials is usually not considered to be magnetic field dependent. Despite this fact, a strong impact of magnetic fields on the intensity and polarization of Raman scattered light has recently been reported for the transition metal dichalcogenide (TMDC) $MoS_2$.[1,2] However, the underlying mechanisms of the oberserved phenomena are presently still a matter of debate. We present results on Raman scattering on related 2D materials as well as other thin films for which similarly remarkable influence of external magnetic fields is revealed. Our studies include also heterostructures containing 2D ferromagnetic materials such as $Fe_{3-5}GeTe_2$ which exhibits above room-temperature ferromagnetism and a perpendicular magnetic anisotropy (PMA). For the such hybrid systems, our results enable a facile way to probe the local magnetic field at the proximity of magnet/nonmagnet interfaces.
[1] Ji et al., PNAS 2016, 113, 9, p. 2349.
[2] Wan et al., RCS Adv. 2021, 11, p. 4035.

HL 40.12 Thu 12:45 EW 201

**Electrical Observation of Skyrmions in the Sandwich Structure Incorporating Intrinsic Ferromagnetic Topological Insulators** — •Takuya Takashiro[1], Ryota Akiyama[1], Ivan Kibirev[2], Andrey Matetskiy[2], Ryosuke Nakanishi[1], Shunsuke Sato[1], Takuro Fukasawa[3], Taisuke Sasaki[4], Haruko Toyama[1], Kota Hiwatari[1], Andrey Zotov[2], Alexander Saranin[2], Toru Hirahara[3], and Shuji Hasegawa[1] — [1]Department of Physics, The University of Tokyo, Tokyo, Japan — [2]Vladivostok, Russia — [3]Department of Physics, Tokyo Institute of Technology, Tokyo, Japan — [4]National Institute for Materials Science, Tsukuba, Japan

A topological insulator (TI) with ferromagnetism exhibits an energy gap at the Dirac point of the topological surface state (TSS), which provides a stage for interesting phenomena such as the quantum anoma-

lous Hall effect and magnetic vortices, skyrmions. In particular, an intrinsic ferromagnetic TI, $Mn(Bi,Sb)_2Te_4$, has been actively studied because of a regularly arranged Mn-monolayer which induces ferromagnetism hybridizing with the TSS. In this study, we electrically observed skyrmions emerging in $Mn(Bi,Sb)_2Te_4$ layers in a sandwich structure of $Mn(Bi,Sb)_2Te_4/(Bi,Sb)_2Te_3/Mn(Bi,Sb)_2Te_4$ and found that skyrmions were stabilized by TSSs by tuning the Fermi level and the $(Bi,Sb)_2Te_3$-thickness. Intriguingly, the highly-ordered Mn monolayers make the skyrmions "soft-magnetic", which is promising for such as rewritable skyrmion memory (T. Takashiro, et al. Nano Lett. 22, 881 (2022)).

## HL 41: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing III (joint session HL/DY/TT/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.

Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Thursday 9:30–13:00 Location: EW 202

**Invited Talk** HL 41.1 Thu 9:30 EW 202
**Quantum sensors and memories based on soft-clamped phononic membrane resonators** — •Albert Schliesser — Niels Bohr Institute, Copenhagen University, Denmark

Soft-clamping of membrane resonators using a phononic pattern enables Q-factors above 1 billion and coherence times exceeding 100 ms at low temperature. We monitor the motion of such membranes with optical interferometry. This allows us to measure force and displacement at and beyond the standard quantum limit, and control the motional quantum state, even at room temperature. This platform lends itself for sensing applications; as an example, we image individual viruses and nanoparticles using the membrane as a force sensor. In a different set of experiments, we demonstrate mechanical storage and subsequent retrieval of optical pulses with an efficiency of 40%, suggesting applications as quantum memory for light.

**Invited Talk** HL 41.2 Thu 10:00 EW 202
**Quantum mechanics-free subsystem with mechanical oscillators** — •Laure Mercier de Lepinay[1], Caspar Ockeloen-Korppi[1], Matthew Woolley[2], and Mika Sillanpää[1] — [1]Department of Applied Physics, Aalto University, P.O. Box 15100, FI-00076 Aalto, Finland — [2]School of Engineering and Information Technology, UNSW Canberra, ACT, 2600, Australia

Quantum mechanics sets a limit on the precision of the continuous measurement of an oscillator's position. However, with an adequate coupling configuration of two oscillators, it is possible to build an oscillator-like subsystem of quadratures isolated from quantum and classical backaction which therefore does not suffer from this limit. We realize such a quantum mechanics-free subsystem using two micromechanical drumheads coupled to microwave cavities. Multitone phase-stable microwave pumping of the system allows to implement the necessary effective coupling configuration. We first demonstrate the measurement of two collective quadratures, evading backaction simultaneously on both of them, obtaining a total noise within a factor of 2 of the full quantum limit. Secondly, this measurement technique is directly adapted to the detection of continuous variable entanglement which is based, according to the Duan criterion, on variance estimates of two collective quadratures. We therefore verify the stabilized quantum entanglement of the two oscillators deeper than had been possible before for macroscopic mechanical oscillators.

**Invited Talk** HL 41.3 Thu 10:30 EW 202
**Electrothermally tunable metal-graphene-siliconnitride membrane mechanical device** — •Elke Scheer, Mengqi Fu, and Fan Yang — Department of Physics, University of Konstanz, 78457 Konstanz

Controlling the properties of mechanical devices over a wide range is important for applications as well as for fundamental research. In this work, we demonstrate an on-chip tunable device composed of a suspended siliconnitride (SiN) membrane with a graphene (G) layer on top which is connected to Au electrodes. Taking advantage of the electrical and thermal conductance properties of G and the difference in the thermal expansion coefficients of SiN and Au, we developed a device in which the G-Au interface serves as local heater by injecting a dc current. The force induced by the thermal expansion difference tunes the residual stress in the SiN membrane and deflects the membrane when the loading power overcomes the threshold to the buckling transition. With this device we realize an extreme large eigenfrequency tuning (more than 50 %) of the vibration mode. By injecting an ac voltage instead, and thus applying a periodic force to the membrane, we achieve strong excitation of the membrane resonator into the nonlinear vibration. This device may act as proof-of-principle for a compact on-chip excitation scheme for multidimensional and composite nanomechanical resonators.

**15 min. break**

**Invited Talk** HL 41.4 Thu 11:15 EW 202
**From Nanomechanics to Spins** — •Christian Degen — ETH Zurich, Switzerland

Nanomechanical resonators are exquisite sensors for weak magnetic forces, with exciting prospects in nanoscale detection and imaging of nuclear and electronic spins. In this talk, I will give an overview of our laboratory's activities in this field, including force detection with optomechanical membranes and strings, and nuclear spin imaging with the technique of magnetic resonance force microscopy.

**Invited Talk** HL 41.5 Thu 11:45 EW 202
**Enhanced cooling efficiency in nonlinear cavity optomechanics** — •Anja Metelmann[1], Nicolas Diaz-Naufal[2], David Zoepfl[3], Lukas Deeg[3], Christian Schneider[3], Mathieu Juan[4], and Gerhard Kirchmaier[3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Free University Berlin, Berlin, Germany — [3]University of Innsbruck, Innsbruck, Austria — [4]Universite de Sherbrooke, Sherbrooke, Canada

Unlocking the quantum potential of mechanical resonators hinges on achieving ground state cooling, a key milestone for quantum information processing and ultra-precise quantum measurements. In the vibrant field of cavity optomechanics, dynamical backaction cooling and feedback protocols have successfully nudged macroscopic mechanical elements toward the quantum ground state. While linear regime cooling is well-explored, recent theoretical insights suggest that a nonlinear cavity could amplify cooling efficiency. We explore this intriguing nonlinear regime, focusing on the cooling dynamics of a mechanical resonator coupled to a nonlinear cavity, embodying the characteristics of a high-Q Duffing oscillator. In this talk we present a comparative analysis between theoretical predictions and experimental results from a magnetomechanical platform. The findings unveil a captivating enhancement in cooling efficiency attributed to the Duffing nonlinearity. This breakthrough not only enriches our understanding of optomechanical interactions but also holds promise for advancing cooling strategies in quantum technologies.

HL 41.6 Thu 12:15 EW 202

**Brillouin scattering selection rules in elliptical optophononic resonators** — •Anne Rodriguez[1,2], Priya Priya[1], Edson Cardozo de Oliveira[1], Abdelmounaim Harouri[1], Isabelle Sagnes[1], Florian Pastier[3], Martina Morassi[1], Aristide Lemaître[1], Loic Lanco[1], Martin Esmann[1], and Daniel Lanzillotti-Kimura[1,4] — [1]Centre de Nanosciences et de Nanotechnologies, Université Paris-Saclay, CNRS, Palaiseau, France — [2]present address: Chair for Nano and Quantum Sensors, Technische Universität München, Garching, Germany — [3]Quandela SAS, Palaiseau, France — [4]Institut für Physik, Universität Oldenburg, Germany

The selection rules of spontaneous Brillouin scattering in bulk crystalline solids are intrinsic material properties that formally constrain the energy, direction and polarization of the scattered photons for a given input state. In this work, we manipulate the polarization states of the input laser and Brillouin signal independently using polarization-sensitive optical micropillar cavities. The ellipticity of the micropillars lifts the degeneracy of the optical cavity modes, and induces a wavelength-dependent rotation of polarization [1,2], altering the Brillouin scattering selection rules. We developed a Brillouin spectroscopy scheme based on polarization filtering, allowing to measure acoustic phonon resonances with frequencies in the range of 20-100 GHz [3], with background-free spontaneous Brillouin scattering spectra.

[1] H. Wang et al., Nat. Phot. 13, 770 (2019). [2] B. Gayral et al., APL 72, 1421 (1998). [3] A. Rodriguez et al., ACS Photonics 10, 1687 (2023).

HL 41.7 Thu 12:30 EW 202

**3D Microwave Cavity-Assisted Detection of High-Q Silicon Nitride Nanomechanical String Resonators** — •Run Fa Jonny Qiu, Anh Tuan Le, Avishek Chowdhury, and Eva Weig — Technical University of Munich, Chair of Nano- and Quantum Sensors, Hans-Piloty Str. 1, 87548 Munich, Germany

Amorphous, low-pressure chemical vapor deposition (LPCVD)-grown silicon nitride (Si3N4) is a highly pre-stressed material due to its thermal-coefficient mismatch and is exploited in our fabrication of doubly-clamped freely suspended nanomechanical string resonators with superjacent electrodes for dielectric drive and detection. High-quality factor (Q-factor) nanomechanical string resonators with a Q-factor of roughly 300000 were fabricated. Two large gold-coated antennas connected to the electrodes are deposited on-chip which permits for a direct coupling of the mechanical displacement-induced change of the capacitance between the electrodes to the electric field of the three-dimensional (3D) rectangular cavity. Research on the quarter-wave coaxial cavity together with a capacitive loop and disk coupling revealed the possibility of both coupling schemes for the detection of mechanical modes. Applying direct current (DC) voltage to the electrodes allows for a frequency tuning of the mechanical flexural modes in the opposite direction, which due to the inherent coupling of the two in-plane (ip) and out-of-plane (oop) modes leads to an avoided crossing.

HL 41.8 Thu 12:45 EW 202

**Optomechanical acceleration beats in confined polariton condensates** — Alexander Kuznetsov, Klaus Biermann, and •Paulo Ventura Santos — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

High-frequency optomechanics involving optoelectronic systems with long temporal coherences enable access to the regime of non-adiabatic modulation, where the optomechanical modulation quantum $\hbar\Omega_M$ exceeds the typical energy decoherence rate of the optoelectronic resonances. Characteristic for this regime is the appearance of modulation sidebands around the optoelectronic resonance line displaced by energy multiples $m\Omega_M$,$(m = 0, \pm1, \dots)$ with amplitude and number determined by the energy modulation amplitude $\Delta E_M$. Here, we experimentally demonstrate a novel regime of temporal coherence invoked by the harmonic modulation of an optomechanical resonance at extreme energy modulation amplitudes $\Delta E_M/(\hbar\Omega_M) > 150$. We show that the resonance energy of a confined exciton-polariton Bose-Einstein condensate harmonically driven at these high relative modulation amplitudes exhibit temporal correlations with timescales much shorter than the modulation period [Kuznetsov et al., DOI:10.21203/rs.3.rs-3197243/v1]. These correlations manifest themselves as comb of spectral resonances with energy scale determined by the ratio $\Delta E_M/(\hbar\Omega_M)$. We show that they arise from accelerated rates of energy change during the harmonic cycle and are, thus, termed the acceleration beats.

## HL 42: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:15 Location: EW 203

HL 42.1 Thu 9:30 EW 203

**Raman spectroscopy on BaTiS3 perovskite nanocrystals** — •Selina Nöcker[1], Sandra Zech[1], Vincent Mauritz[2], Katharina Dehm[2], Ryan Crisp[2], and Janina Maultzsch[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Perovskites and related materials are emerging candidates for photovoltaics demonstrating promising energy conversion efficiencies. Here we study lead- and halide-free BaTiS3, colloidally synthesized as wire- and rod-shaped nanocrystals.

For the structural analysis of those nanocrystals, we use Raman spectroscopy and compare the results to single-crystal spectra of BaTiS3. Our study includes temperature-dependent and excitation-wavelength dependent measurements. Moreover, we show that Raman spectroscopy can be used as a straightforward method to distinguish between the two shape types.

HL 42.2 Thu 9:45 EW 203

**Crystallization and defect properties in combinatorially synthesized $BaZrS_3$ thin films** — •Adriana Röttger[1], Jack Van Sambeek[2], Marin Rusu[1], Hannes Hempel[1], Rafael Jaramillo[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin, Deutschland — [2]Massachusetts Institute of Technology, Cambridge, MA, USA

$BaZrS_3$ is a chalcogenide perovskite composed of Earth-abundant elements with potential applications for photovoltaic (PV) energy conversion. Using pulsed laser deposition, oxide precursors with a lateral [Ba]/[Zr] ratio, ranging from 0.8 to 1.3, were deposited on 50 x 12 $mm^2$ large samples, which were then sulfurized in a tube furnace using different concentrations of $H_2S$ in Ar gas at temperatures ranging from 800°C to 1000°C. The combinatorial nature of the thin films allows the study of crystallization behavior dependent on the composition of the material. A considerable increase in crystallite size was observed from the Zr-rich side to the Ba-rich side of all samples using grazing incidence x-ray diffraction and scanning electron microscopy. We hypothesize that Ba excess leads to liquid phase assisted growth, similar to a low temperature growth mechanism reported recently by Yang et al.[1] We demonstrate control over the kinetics of crystallization by varying temperature and/or $H_2S$ partial pressure. We find that band-edge photoluminescence (PL) increases from the Ba-rich to the Zr-rich side, while defect state PL probed at low temperatures show a reverse trend. This suggests that careful control of the metals ratio will be key to achieving thin films with large crystals and good PV performance.

[1] Yang et al., Chemistry of Materials 2023 35 (12), 4743-4750

HL 42.3 Thu 10:00 EW 203

**Combining transient photoluminescence and transient surface photovoltage experiments: insights from drift-diffusion modeling** — •Orestis Karalis, Hannes Hempel, and Thomas Unold — Helmholtz-Zentrum Berlin, Berlin, Deutschland

The combination of transient surface photovoltage (trSPV) and transient photoluminescence (trPL) can help to distinguish charge transfer and recombination at the interfaces between photo-absorbers and charge-selective layers (I. Levine, 2021). This distinction is particularly crucial for the optimization of halide perovskite solar cells, as their power conversion efficiency is mainly limited by interfacial losses. However rate-equation models previously employed for trSPV (I. Levine, 2021) or trPL (F.Staub, 2016) are unable to simultaneously describe both experiments, which raises concerns about the validity of their findings. To address this limitation, we perform drift-diffusion mod-

eling utilizing the open-source SIMsalabim algorithm (M. Koopmans, 2022). Our investigation reveals that strong charging of the sample with repetitive pulsed illumination, a factor overlooked in previous models, can strongly change the shape of the transients. Based on the improved model, we explore the impact of various parameters, such as charge-transfer velocity, bulk trap density, energy level alignment between absorber and charge transport layer, on the trPL and trSPV transients, as well as on overall solar cell performance. Finally, comparison of these simulations allows a simple phenomenological interpretation of trPL and trSPV. This insight can serve as a valuable guide in the pursuit of optimizing halide perovskite solar cells.

HL 42.4 Thu 10:15 EW 203

**Impact of different substrates and annealing treatments on the formation of fully evaporated perovskite** — •Mohamed Mahmoud[1,2], Martin Bivour[1], Yashika Gupta[1,2], Oussama Er-raji[1,2], and Juliane Borchert[1,2] — [1]Fraunhofer ISE, Freiburg, Germany — [2]University of Freiburg, Freiburg, Germany

Perovskite solar cells have the advantages of a strong absorption edge, defect tolerance, and potential cheap production. In the industry, a great interest is shown towards perovskite-silicon tandem solar cells to overcome the single junction limit. Double-sided textured (micrometer sized pyramid) silicon is commonly produced to decrease reflection losses and improve light trapping. Solution-based processing methods of perovskite on top of the textured silicon showed low conformality, which resulted in shunts and non-working solar cells. To overcome this issue, physical vapor deposition (PVD) is used for the different precursors to conformally coat the perovskite on the silicon pyramids. Therefore, we study distinct vacuum-based methodologies for perovskite processing, specifically the hybrid route and the fully evaporated route. In this study, we investigate the effect of different substrates, that includes different materials and different Si pyramid heights, on the formation of fully evaporated perovskite. The results show that different surfaces (i.e. different materials) affects not only the morphology of the evaporated perovskite, but also the crystal structure. In addition to that, we compare planar Si surfaces to nano structured as well as micro structured on the formation of fully evaporated perovskite.

HL 42.5 Thu 10:30 EW 203

**Room temperature exciton-polaritons in quasi-2D Ruddlesden-Popper perovskites** — •Hamid Pashaei Adl[1,2], Christoph Bennenhei[1], Jens Christian Drawer[1], Lukas Lackner[1], Marti Struve[1], Anthony Ernzerhof[1], Nadiya Matukhno[1], Sigalit Aharon[3], David Cahen[3], Martin Esmann[1], and Christian Schneider[1] — [1]Institute for Physics, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg, Germany. — [2]Instituto de Ciencia de Materiales (ICMUV) Universidad de ValenciaC/Catedrático José Beltrán, 2, Paterna E-46980, Spain. — [3]Weizmann Institute of Science234 Herzl Street, Rehovot 7610001, Israel.

Ruddlesden-Popper (RP) layered perovskites [1] with high oscillator strength and large exciton binding energy are promising materials for photonic applications. The crystalline form of these perovskites can be used as excitonic medium in optical microcavities, allowing for the study of their optical properties in the strong light-matter coupling regime. Here, using angle resolved reflection spectroscopy, we show tunable strong coupling of light modes to mechanically exfoliated quasi-2D RP flakes in an open access microcavity under ambient conditions [2], which is supported by transfer matrix calculations. In ongoing experiments, we introduce structured photonic lattices to the open cavity to study the coupling of the polaritons to tailored topological features and investigate Bose-Einstein condensation.

[1] J. C. Blancon, et al., Nat Nanotechnology 15, 969 (2020). [2] L. Lackner, et al., Nat Commun 12, 4933 (2021).

HL 42.6 Thu 10:45 EW 203

**Predicting Optoelectronic Performance: A First-Principles Analysis of Carrier Recombination in Metal Halide Perovskites** — Utkarsh Singh and •Sergei I. Simak — Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83, Linköping, Sweden

Unveiling the full potential of Metal Halide perovskites (MHPs) for optoelectronic applications depends on understanding factors influencing device performance, specifically the interplay between radiative and non-radiative recombination at various carrier densities. We explore these processes, laying the foundation for enhanced device functionality and tailored design approaches. We implement the calculation of carrier recombination facilitated through direct and phonon-assisted mechanisms via a first-principles approach. Using methods at and beyond the level of density functional theory, we highlight the role of MHP constituents and the contribution of various factors towards carrier dynamics. The primary focus is on MHPs CsPbI3 and its lead-free counterpart CsSnI3, where high radiative and low non-radiative recombination rates are favorable for potential use as LEDs. We reveal how these processes depend on the material's electronic structure, dictating the phase space available for charge carrier interactions [1]. An in-depth understanding of principles governing recombination dynamics, implemented in a predictive framework, may significantly impact advancements in this field.

[1] F. Yuan et al., "Bright and stable near-infrared lead-free perovskite light-emitting diodes", Nature Photonics (2023, accepted).

HL 42.7 Thu 11:00 EW 203

**Additive engineering for high bandgap perovskite absorber for application in triple-junction solar cells** — •Athira Shaji[1], Minasadat Heydarian[1], Maryamsadat Heydarian[1], Patricia S. C. Schulze[1], Juliane Borchert[1,2], and Andreas Bett[1] — [1]Fraunhofer Institute for Solar Energy Systems — [2]INATECH, University of Freiburg

Multi-junction solar cells can overcome the theoretical efficiency limit of state-of-the-art silicon single-junction solar cell. Recently, perovskite-silicon tandem solar cells have achieved high power conversion efficiency (PCE) of 33.9% on small area. By adding a third junction this PCE can be further increased. For a top cell in a triple-junction solar cell, a high band gap (HBG) perovskite is required. However, there are several challenges associated with such HBG perovskites such as photo-induced phase segregation and high $V_{OC}$ deficit[1]. In addition, the high Br content in the HBG perovskite composition has been lead to poor perovskite film formation and morphology which can exacerbate the mentioned issues[1]. Suppression of phase segregation and increased grain size can be achieved by improving the perovskite crystallization via additive engineering[1]. Here, we employ a triple cation perovskite composition with general formula $Cs_{0.05}(FA_{1-x}MA_x)_{0.95}Pb(I_{1-x}Br_x)_3$ ($E_g$ >1.83 eV) which is used as the top cell absorber[2]. We investigate the effects of additives on this perovskite crystallization and grain size[1].

1.Chen, B. et al. Joule 2019, 3(1), 177-190.
2.Heydarian, M. et al. ACS Energy Lett. 2023, 8(10), 4186-4192.

**15 min. break**

HL 42.8 Thu 11:30 EW 203

**Thermodynamics and kinetics of silver in Cu(In,Ga)$Se_2$ solar cell absorbers** — Markus Mock, •Delwin Perera, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Cu(In,Ga)$Se_2$ (CIGS) is at the moment the most efficient absorber material in thin-film solar cells. Its efficiency can be further enhanced by substituting copper with silver which increases the band gap and turns CIGS into a wide-gap semiconductor with potential application in tandem solar cells.

In this contribution, we investigate the impact of silver on structural and electronic properties of CIGS. Using semi-grand canonical Monte Carlo simulations, we explore the CIGS phase diagram as a function of silver content. In particular, we map out the phase transition between solid solution and phase decomposition as well as the spinodal region. Based on a cluster expansion model, our Monte Carlo simulations reveal the microstructure evolution within the binodal region. We supplement the thermodynamic analysis with kinetic considerations by calculating defect migration barriers and defect association energies. Finally, we investigate the effect of silver on the band gap employing hybrid density functional theory calculations.

HL 42.9 Thu 11:45 EW 203

**Photon echo spectroscopy of $CsPbI_3$ nanocrystals** — Artur V. Trifonov[1,2], •Mario Alex Hollberg[1], Stefan Grisard[1], Elena V. Kolobkova[3,4], Maria S. Kuznetsov[2], Mikhail O. Nestoklon[1], Jan Kaspari[5], Doris Reiter[5], Dmitri R. Yakovlev[1,6], Manfred Bayer[1], and Ilya A. Akimov[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund — [2]St. Petersburg, Russia — [3]St. Petersburg, Russia — [4]St. Petersburg, Russia — [5]Condensed Matter Theory, Technische Universität Dortmund — [6]St. Petersburg, Russia

All-inorganic halide perovskite nanocrystals hold potential for future optoelectronic technologies. One of the paths to fully unlock their capabilities, is a deeper understanding of coherent exciton dynamics in these materials. In this work, we investigated a caesium lead tri-iodide ($CsPbI_3$) nanocrystal ensemble using time-resolved photon echo spectroscopy at cryogenic temperatures (1.5 K). We observed a long exciton lifetime $T_1$ of about 1 ns and an exciton coherence time $T_2$ of up to approximately 300 ps. The initial tens of picoseconds in the photon echo decay exhibited oscillatory behavior with two most pronounced frequencies of 3.2 meV and 5.1 meV, which we attribute to the interaction between excitons and optical phonons. The exciton fine structure manifests itself at lower oscillation frequencies of 0.2 meV and 1.1 meV.

HL 42.10 Thu 12:00 EW 203

**Damping the phase segregation in mixed halide perovskites: Influence of X-site anion** — •Maria Azhar — Universitz of Konstanz, Konstanz, Germany

This study reveals that phase segregation becomes more prominent on decreasing bromine content in mixed halide CsPbBr3-xClx perov*skites, when bromine content is 50NCs have been synthesized to mitigate the phase segregation. The grain size of the synthesized NCs exists in the range of 20*25 nm. The selected area electron diffraction exhibits the faint rings of the CsPbBr1.5Cl1.5 indicating the presence of defects in NCs and the X-rays diffraction analysis confirms the NCs exist in monoclinic crystal structure. Mixed halides perovskites have same crystal structure but exhibit a slight shift in $2\theta$ values. The trend in stability follows the order as, CsPbBr3-xClx > CsPbCl3 > CsPbBr3 that is estimated by the values of octahedral factor ($\mu$) and tolerance factor (t). The UV*Vis and steady-state photoluminescence (PL) analysis depict a blue-shift in the spectra by substituting bromine with chlorine in CsPbBr3. The PL kinetics analysis predicts the CsPbBr2.5Cl0.5 exhibits the longest average PL lifetime amongst all other CsPbBr3-xClx perovskites NCs. Our study provides insights in designing stable mixed halides perovskites by suppressing the phase segregation.

HL 42.11 Thu 12:15 EW 203

**Extrinsic doping and compensating defects in the 2D hybrid perovskite $PEA_2PbI_4$** — Gabrielle Koknat[1], Haipeng Lu[2,3], Yi Yao[1], Ji Hao[2], Xixi Qin[1], Chuanxiao Xiao[2], Ruyi Song[1], Florian Merz[4], Markus Rampp[5], •Sebastian Kokott[6], Christian Carbogno[6], Tianyang Li[1], Glenn Teeter[2], Matthias Scheffler[6], Joseph J. Berry[2], David B. Mitzi[1], Jeffrey L. Blackburn[2], Volker Blum[1], and Matthew C. Beard[2] — [1]Duke University, Durham, NC, USA — [2]NREL, Golden, CO, USA — [3]Hong Kong University of Science and Technology, Hong Kong, China — [4]Lenovo HPC Innovation Center, Stuttgart, Germany — [5]MPCDF, Garching, Germany — [6]NOMAD laboratory at FHI, Berlin, Germany

2D hybrid organic-inorganic perovskites are exciting materials for optoelectronic device applications due to their higher chemical and structural adjustability. Precise control over carrier concentrations necessitates the electronic doping of these materials through the incorporation of extrinsic dopants. Conversely, the undesirable presence of intrinsic defects can adversely affect electronic doping efficiencies. In this study, we investigate intrinsic point defects and extrinsic dopants (e.g., Bi, Sn [PRX Energy, 2, 023010 (2023)]) both in isolation and as combined defects in phenylethylammonium lead iodide ($PEA_2PbI_4$). Employing spin-orbit-coupled hybrid density functional theory (DFT) and supercell models scaling up to 3,383 atoms, we identify the anticipated positions of dopant-derived electronic levels within the bandgap. Complementary experimental findings reinforce hypotheses of compensation mechanisms and limiting factors derived from DFT.

HL 42.12 Thu 12:30 EW 203

**Growth and Investigation of Sequentially Evaporated Mixed Halide (Cs,FA)Pb(I,Br)3 Perovskites** — •Tobias Schulz[1], Karl Heinze[1], Paul Pistor[2], and Roland Scheer[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — [2]Universidad de Pablo de Olavide, Carretera de Utrera 1, 41013 Sevilla, Spain

Perovskite films were grown via thermal evaporation and characterized via in situ XRD which give structural information in real-time. Besides the growth of FAPbI3 and (Cs,FA)PbI3 also bromine incorporation into the perovskite to prepare (Cs,FA)Pb(I,Br)3 was investigated [1]. The substitution of iodine with bromine increases the band gap, which is interesting for tandem applications, and improves the thermal stability. In contrast to co-evaporation, the less studied sequential evaporation route was employed which allows a more precise process control. Sequential perovskite formation in vacuum in general proceeds via diffusion of the reactants CsI, FAI, PbI2, and PbBr2 which are assembled in different layer stacks. With the in situ XRD setup, the diffusion of these materials during the necessary annealing step was observed. In combination with SEM images, the reactant's diffusion speed was quantified. Additionally, the perovskites show no unfavourable delta-phase during our experiments, allowing the assumption, that sequential evaporation can fully suppress this non-photoactive phase. [1]: K. Heinze, T. Schulz et al., "Structural Evolution of Sequentially Evaporated (Cs,FA)Pb(I,Br)3 Perovskite Thin Films via In Situ XRD", Physica Status Solidi A, accepted for publication

HL 42.13 Thu 12:45 EW 203

**Impact of ion migration on the performance and stability of perovskite-based tandem solar cells** — •Sahil Shah and Martin Stolterfoht — Physik weicher Materie, Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

Mobile ions play a significant role in perovskite photovoltaics, yet their impact on the overall performance and stability of tandem solar cells (TSCs) remains largely unexplored. In this study, we present a comprehensive study that combines an experimental analysis of ionic losses in Si/perovskite and all-perovskite TSCs, drift-diffusion simulations, and sub-cell-selective measurements on all-perovskite TSCs during aging. Our findings demonstrate that mobile ions have a significant influence on the hysteresis of Si/perovskite tandem solar cells at high scan speeds (400 V/s) during current-voltage measurements, as well as on performance degradation due to field screening. Additionally, subcell-dominated measurements reveal more pronounced ionic losses in the wide-bandgap subcell during aging, which we attribute to its tendency for halide segregation. Drift-diffusion simulations fully corroborate the results. Overall, this work provides valuable insights into ionic losses in perovskite solar cells and discloses new opportunities for their optimization toward more efficient and stable perovskite-based tandem cells.

HL 42.14 Thu 13:00 EW 203

**Why copper oxide is not a reliable hole transporting layer for perovskite solar cells** — •Małgorzata Kot[1], Ludwig Marth[2], Zbigniew Starowicz[3], Paul Plate[2], Jan Ingo Flege[1], and Katarzyna Gawlinska-Necek[3] — [1]APHLS, BTU Cottbus-Senftenberg, Konrad-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH INSTRUMENTS GmbH, Schwarzschildstr. 2, 12489 Berlin, Germany — [3]IMMS PAS, Photovoltaic Laboratory, 22 Krakowska St., 43-340 Kozy, Poland

One approach, among many others, to increase the stability of perovskite solar cells is to replace an organic hole transporting layer (HTL), which becomes highly unstable when exposed to air for a long time, with more stable inorganic materials. The material that seems to be very promising is copper oxide. In our investigation we however found, that the formamidinium lead iodide perovskite deposited directly on copper oxide in the p-i-n structure degrades within tens of minutes due to the migration of copper ions under X-ray exposure and creation of CuI and Cu. Furthermore, an application of an ultrathin atomic layer deposited Al2O3 film on the copper oxide substrate, that in our previous work [1] succesively blocked the migration of perovskite ions into the HTL in the n-i-p structure, does not sufficiently block the migration of copper ions through the perovskite film. Therefore, in order for copper oxide to be a reliable HTL for perovskite solar cells, an effective method must be still developed to block the migration of copper ions into other layers. [1] C. Das et al., Cell Rep. Phys. Sci. 2020, 100112.

# HL 43: Optical Properties II

Time: Thursday 9:30–11:45 Location: EW 561

HL 43.1 Thu 9:30 EW 561

**Polarized room-temperature polariton lasing in elliptical microcavities filled with fluorescent proteins** — •Marti Struve[1], Christoph Bennenhei[1], Sven Stephan[1,2], Nils Kunte[1], Victor N. Mitryakhin[1], Falk Eilenberger[3], Jürgen Ohmer[4], Utz Fischer[4], Martin Silies[2], Christian Schneider[1], and Martin Esmann[1] — [1]Institute for Physics, Carl von Ossietzky University of Oldenburg, Germany — [2]University of Applied Sciences Emden/Leer, Germany — [3]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena — [4]Department of Biochemistry, University of Würzburg, Germany

Excitons in organic semiconductors can couple strongly to cavity photons forming exciton polaritons at ambient conditions. In artificial photonic potentials they are an emerging platform to study polariton lasing and Bose-Einstein condensation [1,2]. In this work, we study the polarization properties of fluorescent proteins enclosed by distributed Bragg reflectors with elliptical indentations [3]. We show experimentally and numerically that the structural anisotropy of the elliptical potential and the internal TE-TM splitting of dielectric Bragg reflectors leads to a distinct polarization splitting. This splitting enforces condensation into one polaritonic mode with linear polarization. Our devices have relevant applications for the engineering and tuning of polarization in room temperature polariton lasers through additional degrees of freedom. References [1] S. Betzold et al. ACS Photonics 7, 384 (2020). [2] M. Dusel et al. Nano Lett. 21, 6398 (2021). [3] C. Bennenhei, M. Struve et al. Opt. Mater. Express 13, 2633 (2023).

HL 43.2 Thu 9:45 EW 561

**Optical realization of Shubnikov - de Haas and other quantum oscillations in THz transmission** — •Maksim Savchenko — Vienna University of Technology

Due to causality-related correspondence between static and dynamic properties of physical systems, quantum oscillation observed in a DC response must reveal their counterpart in the optical domain.

In the talk, I will present the optical analogues of three types of the DC transport quantum oscillations. First, the optical realization of the microwave-induced resistance oscillations that are measured in the optical response, sub - terahertz transmittance of a two-dimensional system [1]. Second, the optical counterpart of the transport Shubnikov - de Haas oscillations, where we reveal two distinct types of oscillation nodes: 'universal' nodes at integer ratios of radiation and cyclotron frequencies and 'tunable' nodes at positions sensitive to all parameters of the structure. We analyse the nodes in both real and imaginary parts of the measured complex transmittance using a dynamic version of the static Lifshitz-Kosevich formula. And third, I will present the optical oscillations that have the same origin as transport magneto-intersubband oscillations.

These results reveal another advantage of the optical studies that provide a simultaneous access to quantization- and interaction-induced renormalization effects. And in conclusion, I will also discuss current opportunities and challenges to observe other well-known in DC transport effects in the optical domain.

[1] M. L. Savchenko et al., PRR 3, L012013 (2021).

HL 43.3 Thu 10:00 EW 561

**Coherence of magnetic-field-coupled $1S$ excitons in $Cu_2O$** — •Andreas Farenbruch[1], Nikita V. Siverin[1], Gülistan Uca[1], Dietmar Fröhlich[1], Heinrich Stolz[2], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]TU Dortmund, Dortmund, Germany — [2]Universität Rostock, Rostock, Germany

The coherence of the $1S$ exciton state in cuprous oxide ($Cu_2O$) is investigated using difference frequency generation with two-photon excitation (2P-DFG) for varying temperatures and excitation powers. The pulses of the first laser induce a coherent exciton population via a two-photon excitation process. The pulses of the second laser stimulate the emission of photons with the energy difference between the excitons and the stimulating photons. By delaying the pulses of the second laser, the 2P-DFG signal is measured as a function of time. This technique is used to measure the coherence times of the magnetic-field coupled $1S$ exciton states at magnetic fields of up to 10 T in Voigt configuration.

Characteristic polarization selection rules for this process are derived through group theoretical considerations and experimentally confirmed by measuring the full polarization dependence. Chosen linear polarization settings allow for a selective measurement of the decay of a single exciton state or additional two- or three-level quantum beats. The dependence of the coherence times is investigated for temperatures in the range of 1.4 to 2 K and excitation powers between 3 and 30 mW.

HL 43.4 Thu 10:15 EW 561

**Intensity modulation of a light beam by excitation of 1S-excitons in $Cu_2O$ in a cavity** — •Simon Siegeroth, Binodbihari Panda, Mariam Harati, Julian Heckötter, and Marc Assmann — Department of physics, TU Dortmund, Dortmund 44227, Deutschland

Excitons in Cu2O are a suitable platform to study Rydberg physics. By reaching a high principal quantum number up to 25[1], many characteristic properties increase by orders of magnitude compared to ground state excitons, such as the radius ($r \propto n^2$), the lifetime ($t \propto n^3$) or the blockade volume ($V \propto n^7$). Here we report on the interaction between Rydberg excitons and ground state excitons (1S). By exciting 1S-exctions via a two-color pump probe setup we observed modulation of the laser intensity of the transmitted probe beam in spectral dependency. The modulation is dependent on pump laser energy & power and also visible in the reflected probe beam. This phenomenon is investigated for a set of parameters such as pump-power, angle, probe-polarization, probe-power and overlap. The oscillations do only appear when the sample is mounted strain free between two glass plates with a low reflectivity of around 4% at each surface which are forming a (bad) cavity. Interestingly the oscillations appear as well when the probe laser is tuned out of resonance.

[1] T. Kazimierczuk, D. Fröhlich, S. Scheel, H. Stolz, and M. Bayer. "Giant Rydberg excitons in the copper oxide Cu2O." Nature 514 (2014), pp. 343-347.

**15 min. break**

HL 43.5 Thu 10:45 EW 561

**Organic room-temperature polariton condensate in a higher-order topological lattice** — •Christoph Bennenhei[1], Hangyong Shan[1], Marti Struve[1], Nils Kunte[1], Falk Eilenberger[2], Jürgen Ohmer[3], Utz Fischer[3], Xuekai Ma[4], Christian Schneider[1], and Martin Esmann[1] — [1]Institute of Physics, Universität Oldenburg, Germany — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany — [3]Department of Biochemistry, Universität Würzburg, Germany — [4]Department of Physics, Paderborn University, Germany

Organic molecule exciton-polaritons in artificial photonic lattices have emerged as a versatile platform to emulate unconventional phases of matter at ambient conditions, including protected interface modes in topological insulators [1]. We investigate bosonic condensation in the most prototypical higher-order topological lattice, a 2D-version of the Su-Schrieffer-Heeger (SSH) model, which supports both zero- and one-dimensional topological defect modes. Using spatially resolved photoluminescence spectroscopy, we observe the topological defect modes of fluorescent protein-filled distributed Bragg reflector cavities with a fabricated lattice of hemispherical indentations defining a staggered photonic trapping potential. We observe bosonic condensation into topologically protected interface modes and demonstrate spatial first-order coherence in the protected 1D channels via interferometric measurements. Our findings pave the way towards organic on-chip polaritonics using higher-order topology as a tool for the generation of robustly confined lasing states. [1] Nano Lett. 2021, 21, 15, 6398-6405

HL 43.6 Thu 11:00 EW 561

**Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation** — •Pier Luigi Cudazzo — University of Trento (Italy)

One of the big challenges of theoretical condensed matter physics is the description, understanding, and prediction of the correlation effects induced by the mutual interaction between particles on materials properties. In both electronic and optical spectra the Coulomb interaction and the electron-phonon coupling cause a renormalization of the energies and change of spectral weight. Most importantly, they induce

a finite lifetime on the quasi-particle (QP) excitations and can lead to new structures, often called satellites. The latter are pure many body effects and can be linked to the coupling of excitations, also termed dynamical effects. Standard methods developed in the framework of many body perturbation theory namely GW and the Bethe-Salpeter equation (BSE) are often not able to capture this complex physics. Instead, approaches based on a picture of electron-boson coupling such as the cumulant expansion are promising for the description of plasmon and phonon satellites. Motivated by the recent success of the cumulant expansion of the one particle Green's function in the description of photoemission spectra, we generalized the cumulant approach to the evaluation of the electronic polarizability. In this way we provide a new full ab-initio tool to include dynamical effects beyond the standard BSE in the description of neutral excitations as measured in optical absorption, photoluminescence, electron energy loss and inelastic X-rays scattering spectroscopies.

HL 43.7 Thu 11:15 EW 561

**Hyper-Raman effect on magnetic-field coupled $1S$ exciton polaritons in $Cu_2O$** — •Gülistan Uca[1], Andreas Farenbruch[1], Dietmar Fröhlich[1], Heinrich Stolz[2], Dmitry Yakovlev[1], and Manfred Bayer[1] — [1]TU Dortmund, Dortmund, Germany — [2]Universität Rostock, Rostock, Germany

We analyzed the polarization dependence of the hyper-Raman effect for magnetic field-coupled $1S$ exciton polaritons in cuprous oxide ($Cu_2O$), a material recently recognized for hosting Rydberg excitons with high principal quantum numbers. The hyper-Raman effect is a coherent process consisting of a two-photon excitation on the polariton branch and an emission of both a phonon and a photon. Characteristic polarization selection rules for this process are derived through group theoretical considerations. Applying this approach, the full polarization dependence of this process was simulated and measured for the hyper-Raman effect at a magnetic field of 10 T in Voigt configuration involving the $\Gamma_3^-$ phonon. Further investigations focused on the hyper-Raman effect with a sideband emission involving the $\Gamma_5^-$ phonon, as well as the longitudinal-transverse split $\Gamma_4^-$ phonon mode.

HL 43.8 Thu 11:30 EW 561

**Phonon-phonon interactions in the polarization dependence of Raman scattering** — •Nimrod Benshalom[1], Noam Pinsk[1], Maor Asher[1], Olle Hellman[2], and Omer Yaffe[1] — [1]Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Rehovot 76100, Israel

Inelastic light scattering offers an experimentally robust and accessible method to probe the potential surface governing ionic motion in crystals. Its analysis, however, usually relies on harmonic theory that predicts Lorentzian line shapes, monotonic temperature trends and strict selection rules. Since the spectra of dynamically disordered crystals can violate all of these, new evaluation schemes are required to realize the potential for physical insight dormant in light scattering experiments.

We have found that the polarization dependence of Raman scattering in organic crystals at finite temperatures can only be described by a fourth-rank tensor formalism. This generalization of the second-rank Raman tensor stems from the effect of off-diagonal components in the crystal self-energy on the light scattering mechanism. We thus establish a novel manifestation of phonon-phonon interaction in inelastic light scattering, markedly separate from the better-known phonon lifetime.

## HL 44: Nitrides: Preparation and characterization II

Time: Thursday 14:00–17:00 Location: EW 015

HL 44.1 Thu 14:00 EW 015

**Low-temperature plasma-enhanced atomic layer deposition of tunable cobalt nitride thin films** — •Lukas Alexander Kohlmaier[1,2], Matthias Kuhl[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

Transition metal nitrides are an interesting class of materials due to their high mechanical hardness, as well as magnetic and catalytic properties. In this context, cobalt nitride is especially promising for applications in the semiconductor industry and for electrochemical energy conversion. However, the synthesis of uniform cobalt nitride thin films with controlled composition by atomic layer deposition (ALD) is still rather unexplored. Here, we deposit cobalt nitride thin films by plasma-enhanced (PE) ALD using a cobaltocene precursor. Specifically, we analyzed the impact of different co-reactants and their combinations, as well as deposition temperatures, on the growth characteristics and material properties. The deposition at low temperatures ($<$ 200 °C) is only enabled by introducing an additional nitrogen plasma pulse at the end of each PE-ALD cycle to regenerate surface sites for the subsequent precursor adsorption. Increasing deposition temperatures can be leveraged to tune the Co/N ratio and thus the material properties from semiconducting to metallic. Overall, this work puts forward PE-ALD as a promising approach for tuning the material properties of metal nitrides.

HL 44.2 Thu 14:15 EW 015

**High temperature growth of cubic gallium nitride by PAMBE** — •Pascal Mahler[1], Dirk Reuter[1,2], and Donat J. As[1] — [1]Paderborn University, Department of Physics, Warburger Strasse 100, 33098 Paderborn — [2]Institut für Photonische Quantensysteme (PhoQS), Warburger Strasse 100, 33098 Paderborn

State of the art cubic gallium nitride layers when grown using plasma assisted molecular beam epitaxy (PAMBE) are usually deposited at a substrate temperature of around 720°C under slightly gallium rich conditions with one monolayer gallium present on the surface during growth. This allows to grow layers with <1% hexagonal GaN content and a roughness of 2-5nm. However, it was shown that for selective area growth of c-GaN higher substrate temperatures of at least 870°C are necessary and that growth of c-GaN can be stabilized at this temperature. Based on these findings, growth of c-GaN on un-patterned 3C-SiC (001) substrates at temperatures from 720°C to 900°C has been investigated. HRXRD measurements reveal that samples grown at a substrate temperature of 860°C showed a decrease in the $\omega$-FWHM of the (002) c-GaN reflection compared to samples optimized for growth at 720°C which according to the Ayers model is linked to a decrease in dislocation density.

HL 44.3 Thu 14:30 EW 015

**uniform large-area top-down GaN nanowire array fabrication with independently tunable diameter and spacing** — •jingxuan kang, rose-mary jose, thomas auzelle, oliver brandt, and lutz geelhaar — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

Top-down approaches to nanowire fabrication offer advantages in controllability over bottom-up growth. However, achieving large-area nanoscale patterning with high throughput poses challenges. This study explores the use of nanoislands resulting from the dewetting of a metal film as mask for GaN nanowire fabrication. To optimize size and shape homogeneity, we have extensively varied the annealing conditions for Pt films of different thicknesses. A thermodynamic model accurately describes the experimental dependencies of island diameter and density on film thickness, as well as the linear relation between island spacing and diameter.

To overcome the fixed spacing-diameter relation imposed by dewetting, we employ digital etching of the GaN nanowires fabricated with the above islands. $O_2$ plasma oxidation followed by KOH wet etching enables a precise reduction of the nanowire diameter, increasing at the same time the spacing. Hence, additional freedom is gained for tailoring the nanowire array properties. Combining metal dewetting with controlled lateral nanowire etching offers a pathway for large-scale top-down nanowire fabrication with both high throughput and flexibility in dimension control.

HL 44.4 Thu 14:45 EW 015

**Metal modulated growth of cubic InGaN by Molecular Beam**

**Epitaxy** — •Silas A. Jentsch[1], Mario F. Zscherp[1], Nicolai M. Gimbel[1], Anja Henss[2], Donat J. As[3], Sangam Chatterjee[1], and Jörg Schörmann[1] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany — [3]Department of Physics, University Paderborn, Germany

Cubic InGaN alloys are candidate materials for next-generation optoelectronic applications as they lack internal fields and promise to cover large parts of the electromagnetic spectrum from the deep UV towards the mid infrared. However, there still exist many challenges with the growth of indium-bearing cubic nitrides. Here we apply a metal-modulated growth approach to improve the morphological and structural quality of the epitaxially grown nitride films as compared to the conventional growth in molecular beam epitaxy.

We report cubic InGaN layers (x(In) = 0.27) grown by metal-modulated plasma-assisted molecular beam epitaxy on c-GaN/AlN/3C-SiC/Si templates which should nominally causes the formation of alternating GaN and InN layers. Surprisingly, we found the formation of a InGaN/GaN superstructures for short InN growth times and a complete mixture of GaN and InN resulting in homogeneous c-InGaN layers for long InN growth times. High-resolution X-ray diffraction (HR-XRD), Atomic Force Microscopy (AFM) and photoluminescence studies reveals the structural and optical properties of our c-InGaN layers.

HL 44.5 Thu 15:00 EW 015

**Molecular beam epitaxy of (Al,Sc)N nanowires** — •Philipp John, Oliver Brandt, Achim Trampert, Lutz Geelhaar, and Thomas Auzelle — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

To extend the functionalities of classical III-nitride devices, combinations with transition metal nitrides are sought. Alloying AlN with ScN, for instance, can enhance its piezoelectric coefficient by up to a factor of 5, provided that the hexagonal wurtzite phase is maintained. Wurtzite (Al,Sc)N is thus a promising material for new types of surface/bulk acoustic devices, piezoelectric energy harvesters and high electron mobility transistors.

In this contribution, we demonstrate (Al,Sc)N growth on self-assembled AlN and GaN nanowire stems by molecular beam epitaxy for a wide range of concentrations. Wurtzite (Al,Sc)N is stabilized at low to moderate Sc concentrations, while a phase transition to the cubic rocksalt structure is found for high Sc concentrations. We will discuss the possibility of growing either axial or core/shell nanowire structures, depending on the (Al,Sc)N growth conditions. Axial nanowire structures offer the preferred geometry for piezoelectric devices, while core/shell nanowires are promising for realizing heterostructures combining group III-nitrides and transition metal nitrides.

HL 44.6 Thu 15:15 EW 015

**Alloying and demixing in AlGaN/GaN nanowire heterostructures** — •Rudolfo Hötzel[1], Lukas Lübken[1], Anton Schäning[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, University of Bremen, 28359 Bremen, Germany

Contrary to common knowledge that GaN nanowires (NW) only grow in the nitrogen-rich (N-rich) regime, a precise evaluation of the growth stoichiometry on the growth surface shows a growth window extending into the metal-rich regime. The AlGaN/GaN NW heterostructures grown by molecular beam epitaxy were analyzed by scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDX) as well as X-Ray diffraction (XRD). In that line, the influence of the III/V-ratio on the alloy formation of the ternary material for N-rich as well as metal-rich growth conditions is studied. In N-rich growth conditions the concentration in the alloy follows a linear trend up to close to the stoichiometric point of GaN, where the increased presence of Al leads to a change of surface adsorption which tips the growth over to the metal-rich regime, where we observe instantaneous growth of pure AlN despite the available Ga flux. However, after some time the growth switches over to incorporate Ga, forming an AlGaN alloy. In other words, even though Al possesses a higher reaction enthalpy and AlN forms, Ga accumulates on the growth surface resulting in another tip-over of the growth regime leading to AlGaN formation.

**15 min. break**

HL 44.7 Thu 15:45 EW 015

**Highly spatially resolved investigation of structural and optical properties of a GaN-based p-n-diode** — •Luca Greczmiel, F. Bertram, G. Schmidt, P. Veit, H. Eisele, A. Dempewolf, S. Petzold, J. Christen, A. Strittmatter, and A. Dadgar — Otto-von-Guericke-University Magdeburg, Magdeburg, Germany

GaN based devices are promising candidates for the next generation of high power electronics due to its high breakdown voltage, high electron mobility and highthermal conductivity. To understand the physics of these complex devices, the fundamental structural, electronic and material properties have to be investigated. In this study, we investigated a GaN based p-n-structure by cathodoluminescence microscopy (CL) directly performed in a scanning transmission electron microscope (STEM). The diode was grown by metal organic vapor phase epitaxy on top of an optimized template. An n-doped GaN layer with nominal 8x$10^{18}$ $cm^{-3}$ Si doping serves as current spreading layer. The p-n-junction is formed by a 970 nm thick GaN:Si layer and a 280 nm GaN:Mg layer with nominal doping concentration of 7x$10^{17}$ $cm^{-3}$ and 1-3x$10^{19}$ $cm^{-3}$, respectively. In scanning electron micrsocopy images, we were able to determine the thickness of the GaN:Mg layer to 280 nm due to the distinct doping contrast. In STEM-CL linescans, we observe a drastic change of the recombination channels. The donor bound exciton emission is dominant at 357.2 nm in the n-GaN layer. Towards the p-n-junction, donor-acceptor-pair recombination (DAP) increases mono-exponentially in intensity and reaches its maximum at the p-n-interface.

HL 44.8 Thu 16:00 EW 015

**Optical and chemical characterisation of $In_xGa_{1-x}N$ layers and nanowire arrays** — •Aidan Campbell, Mikel Gómez Ruiz, Jingxuan Kang, Lutz Geelhaar, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Germany

$In_xGa_{1-x}N$ is an alloy with promising applications in solar water splitting, $CO_2$ conversion, and solar energy harvesting. Particular advantages are the tunable direct bandgap (0.7–3.5 eV), large absorption coefficient ($10^5$ $cm^{-1}$) and high mobility. In this study, we investigate $In_xGa_{1-x}N$ layers of nominal composition $0.025 < x < 0.12$ grown by plasma-assisted molecular beam epitaxy. A multi-spectroscopic approach is employed using cathodoluminscence and energy dispersive X-ray spectroscopy in a scanning electron microscope. Thereby, the chemical, optical, and structural properties can be analysed and correlated for the same local region of a specimen. Factors such as dislocation density, luminous intensity, spatial homogeneity of the composition, and the morphology will be discussed, as they are key properties in optimizing growth techniques enabling high efficiency devices. The dislocation density increases by a factor of 6 over this compositional range, reaching $1.5 \times 10^9$ $cm^{-2}$ at $x = 0.12$. Compositional variations are evidenced by the spatial distribution of emission energies, which for different samples suggest local in-plane variations of $\Delta x = \pm 0.005$–0.008. Finally, the investigation is extended to $In_xGa_{1-x}N$ nanowires obtained from these layers by top-down processing.

HL 44.9 Thu 16:15 EW 015

**MBE growth of cubic InxGa1-xN over the entire GaN/InN composition range** — •Mario F. Zscherp[1], Silas A. Jentsch[1], Marius J. Müller[1], Vitalii Lider[2], Celina Becker[2], Limei Chen[1], Mario Littmann[3], Falco Meier[3], Andreas Beyer[2], Detlev M. Hofmann[1], Donat J. As[3], Peter J. Klar[1], Kerstin Volz[2], Sangam Chatterjee[1], and Jörg Schörmann[1] — [1]Institute of Experimental Physics I and Center for Materials Research, Justus-Liebig-University Giessen — [2]Materials Science Center and Faculty of Physics, Philipps-University Marburg — [3]Department of Physics, University Paderborn

Cubic InxGa1-xN is a candidate material for optoelectronic applications because they lack internal fields and promise to cover a vast range of emission wavelengths. However, the large discrepancy in interatomic spacing and growth temperatures of GaN and InN hinder the growth of c-InxGa1-xN with x(In) > 0.3. Several publications even report spinodal decomposition for intermediate In contents.

We overcome this perceived miscibility gap of c-GaN and c-InN using molecular beam epitaxy. The c-InxGa1-xN layers are grown on smooth c-GaN/AlN/3C-SiC/Si templates. Reciprocal space maps precisely monitor the composition, phase purity, and strain relaxation of the thin films. The photoluminescence data clearly demonstrate the

full tunability of the emission energy from 0.71 to 3.24 eV. Furthermore, scanning transmission electron microscopy, photoluminescence data, and Raman spectroscopy infer a CuPt-type ordering for intermediate In contents as well as short-range ordering for all compositions.

HL 44.10 Thu 16:30 EW 015

**Influence of Surface and Subsurface Damage on GaN Wafer Processing and Laser Facet Fabrication** — •Saad Makhladi — Ferdinand-Braun-Institut (FBH), Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Backside wafer thinning is an inherent part of the process chain to fabricate diode laser chips, enabling precise wafer cleavage with a high structural quality of the laser facets. However, in the case of gallium nitride (GaN) wafers, their brittleness poses challenges for process control, limiting the process yield. To optimize the backend processing of GaN ridge waveguide laser chips, GaN laser wafers underwent backside thinning employing two different technologies, namely lapping and grinding. The laser chips from these wafers were compared. The investigation included a detailed evaluation of backside surface morphology, wafer edge conditions, and subsurface damage (SSD), with respect to crystallinity, stress and wafer bow. As a result of this study, the probability of unintentional breakage of the wafers during processing has been reduced by a factor of two. The bow radius of thinned chips increases from 0.35 m to 0.65 m, and the depth of the SSD is reduced from 2.1 m to 0.8 m by employing Grinding instead of lapping. Certain wafer backside features were found to lead to cracks, which have the potential to propagate during cleavage to enhance terrace formation. i.e., to reduce the facet quality. Further investigations involve subsequent polishing of the GaN wafer backside and studying its impact on the facet formation of GaN Lasers.

HL 44.11 Thu 16:45 EW 015

**HfN as conductive buffer for GaN epitaxy** — •Christopher Lüttich, Florian Hörich, Jürgen Bläsing, André Strittmatter, and Armin Dadgar — Otto-von-Guericke Universität, Magdeburg

Hafniumnitrid-Schichten wurden mittels eines reaktiven DC magnetron Sputterprozess auf Si gewachsen unter verschiedenen Bedingungen. Diese Schichten wurden mit Galliumnitrid überwachsen, mit dem Ziel, vertikale Leitfähigjeit vom Substrat durch die Pufferschicht zum Galliumnitrid zu erreichen.

## HL 45: Materials and Devices for Quantum Technology II (joint session HL/QI)

Time: Thursday 14:00–16:45 Location: EW 203

**Invited Talk** HL 45.1 Thu 14:00 EW 203

**Compact, plug-and-play module to generate high-quality photon states from quantum dots** — •Vikas Remesh — Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

As the quantum revolution gathers pace, there is a constant need to develop novel architectures to control quantum systems. Semiconductor quantum dots (QD) are regarded as the most promising sources of quantum light, due to their wavelength-tunability, high purity, high degrees of entanglement, and scalability. To realize a resource-efficient and scalable platform, it is desirable to have an ensemble of quantum dots that can be collectively excited with high efficiency. Shaped laser pulses have been remarkably effective in the development of controllable quantum systems. The most efficient optical excitation method of quantum dots relies on chirped laser pulses, as it offers robustness against spectral and intensity fluctuations. Yet, the existing methods to generate chirped laser pulses coupled to a quantum emitter are lossy and mechanically unstable, severely hampering the prospects of a practical quantum dot device. In this talk, I will briefly navigate through the impact of pulse-shaping schemes in advancing quantum dot control. Subsequently, I will present a compact, robust, and plug-and-play architecture for chirped pulse excitation of quantum dots, and demonstrate high-quality photon generation. Our method is a significant milestone in realizing a direct fiber-coupled, multipurpose quantum dot photon source.

HL 45.2 Thu 14:30 EW 203

**Light-matter correlations in Quantum Floquet Engineering** — •Beatriz Pérez-González[1], Gloria Platero[1], and Álvaro Gómez-León[2] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spanien — [2]Instituto de Física Fundamental (IFF-CSIC), Madrid, Spanien

Quantum Floquet engineering requires a proper gauge-invariant description of light-matter interaction to correctly capture the physics of the system beyond the strong-coupling regime. This means that such models typically involve a highly non-linear dependence on the photonic operators which makes their analysis and simulation complex.

In this talk, we present a non-perturbative truncation scheme for the light-matter Hamiltonian, which is valid for arbitrary coupling strength. This method can successfully capture the physics of both, fermions and photons, in agreement with the predictions of gauge-invariant models. Importantly, it also keeps track of the role of light-matter correlations, which are essential to correctly predict the properties of the many-body system.

We find that, even in the high-frequency regime, light-matter correlations can spontaneously break key symmetries. We focus on the implications this has when the electronic system has topological properties, since the breaking of a certain symmetry can jeopardize topological properties and their robustness. We exemplify our findings with the SSH chain, and show that a topological phase transition can be induced by coupling to a cavity and that the critical point can be predicted from the spectral function.

HL 45.3 Thu 14:45 EW 203

**Near-Ideal Room Temperature Single Photon Emitters hosted in hexagonal Boron Nitride for Quantum Optics Application** — •Tjorben Matthes[1,2], Anand Kumar[2], Chanaprom Cholsuk[1,2], Mohammad Nasimuzzaman Mishuk[2], Josefine Krause[2], Mouli Hazra[2], Kabilan Sripathy[2], and Tobias Vogl[1,2] — [1]Technical University of Munich, TUM School of Computation, Information and Technology, Arcisstraße 21, 80333 München — [2]Friedrich Schiller University Jena, Institute of Applied Physics, Albert-Einstein-Straße 15, 07745 Jena

In this talk, we will give an insight into our work done on single photon emitters hosted in hexagonal Boron Nitride (hBN) and the integration of those emitters into integrated photonics chips that have laser-written waveguides with controllable crosslinks at their heart.

We recently demonstrated the deterministic creation of identical single-photon emitters in hexagonal Boron Nitride that show exceptional characteristics regarding purity, stability, and brightness. In a follow-up work, we determined additional optical characteristics and carefully compared them to those predicted for numerous defect complexes by density functional theory (DFT) calculations. Currently, we are extending this work, bringing us closer to understanding the actual nature of the defect creation.

Furthermore, we are working on the technical utilisation of single photon emitters for quantum communication and optical circuits. In particular, we focus on laser-written waveguides that can be used for numerous applications having crosslinks with tunable splitting ratios.

HL 45.4 Thu 15:00 EW 203

**Theory of optical ionization of Silicon Vacancies in 4H-SiC** — •Maximilian Schober and Michel Bockstedte — Institute for Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

The Silicon Vacancy ($V_{Si}$) in 4H-SiC represents a quantum bit with advantageous properties for applications like quantum sensing and as a single-photon emitter. Optical readout of its spin state is achieved via a spin-selective optical cycle enabled by coupled defect electron spins and associated spin-dependent interactions. An alternative readout method involves spin-to-charge conversion through optical ionization [1] of the qubit, followed by the electrical detection of the resulting spin-sensitive photocurrents. Relatively little is known, however, regarding the photophysics of the optically silent charge states of $V_{Si}$ created throughout this process. To tackle this issue, we investigate such systems with a combined ab initio framework of density functional theory and CI-cRPA [2] capable of including the crucial multiplet physics of such qubit centers. We discuss the relevant single and two-photon

processes for optical charge state switching and electrical detection of the spin states. Furthermore, we shine light on the nominally "dark" neutral and doubly negatively charged centers as potential infrared emitters.

[1] M. Niethammer et al., Nat Commun 10, 5569 (2019).
[2] M. Bockstedte et al., npj Quant Mater 3, 31 (2018).

**15 min. break**

HL 45.5 Thu 15:30 EW 203

**Inhomogenous broadening of donor bound exciton transitions in ultra-pure 28-Si:P** — •Nico Eggeling[1], Finja Tadge[1], Dolores García de Viedma[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 offer distinct characteristics which qualify them as well-suited candidates for applications in the field of quantum computing [1]. Using a combination of numerical and analytical calculations, we analyze the influence of statistical electric field fluctuations on donor-bound excitonic transitions in ultra-pure 28-Si:P. Our results show good agreement with current measurements of the inhomogeneously broadened excitonic linewidth. Employing approximations concerning screening effects and Monte-Carlo-type simulations, linewidth predictions are made and confirmed. The inhomogeneous nature of the excitonic complex is shown using spectral hole burning [2]. The next steps include measurements and discussion of temporal broadening of the hole-burning linewidth due to donor-acceptor recombination.

[1] Sauter, et al. Phys. Rev. Lett. **126**, 137402, (2021).
[2] Yang, et al. Appl. Phy. Lett. **95**, 122113, (2009).

HL 45.6 Thu 15:45 EW 203

**All-dry Pick-Up and Transfer Method for Quantum Emitters in hBN** — •Mohammad Nasimuzzaman Mishuk[1,2], Mouli Hazra[2], Anand Kumar[1,2], and Tobias Vogl[1,2] — [1]Department of Computer Engineering, School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [2]Abbe Center of Photonics, Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany

Quantum emitters (QE) hosted by defects in hexagonal Boron Nitride (hBN) can operate at room temperature, serving as stable single photon emitters. They can also be integrated into various materials and devices, making them highly versatile in quantum technologies and photonic integrated circuits. However, creating these quantum emitters directly on different surfaces is challenging. That's why more often they are created on standard silicon chip coated with thin silicon dioxide layer. Owing to this difficulty, various transfer processes are developed which are mostly wet. In this study, we present an all-dry transfer method for transferring quantum emitters onto arbitrary substrates. Using our pick-up and transfer method, we have achieved a success probability of 1 in 4 for any single photon emitter. The validity of our results has been confirmed through second-order correlation measurements. We are actively working on improving its quality, quantity, and accuracy.

HL 45.7 Thu 16:00 EW 203

**Plug-and-play quantum light from semiconductor quantum dots in fiber-pigtailed hybrid circular Bragg Gratings** — •Lucas Rickert[1], Kinga Zolnacz[2], Daniel Vajner[1], Martin v. Helversen[1], Johannes Schall[1], Shulun Li[1,4], Sven Rodt[1], Anna Musial[3], Grzegorz Sek[3], Zhichuan Niu[4], Stephan Reitzenstein[1], 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

We report on the fabrication of hybrid circular Bragg gratings (hCBGs) with deterministically integrated semiconductor quantum dots (QDs), and discuss in detail the fabrication methods to deterministically match the emitter spatially and spectrally to the cavity mode. The devices exhibit bright, pure and indistinguishable single photon emission with experimentally measured Purcell enhancement >15 with high reproducibility.

Finally, we show how these high-performance hCBGs can be combined with directly attached single-mode fibers to harness the high quality quantum light in a plug-and-play fashion, and discuss excitation schemes suitable for optimum performance of these fiber-coupled systems.

HL 45.8 Thu 16:15 EW 203

**Optical dipole orientation of single photon emitters in $MoS_2$** — •Katja Barthelmi[1,2], Lukas Sigl[1], Tomer Amit[3], Mirco Troue[1], Thomas Klokkers[1], Anna Herrmann[1], Takashi Taniguchi[4], Kenji Watanabe[4], Sivan Refaely-Abramson[3], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physik Department, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Weizmann Institute of Science, Revohot, Israel — [4]National Institute for Materials Science, Tsukuba, Japan

Single photon emitters in monolayer $MoS_2$ can be formed by helium ion irradiation. The irradiation results in defects with an emission energy of 1.75 eV and a high position accuracy [1-3]. To further understand the microscopic structure of the defects, we study their emission dipole orientation by back focal plane imaging. We find that the optical dipole of the quantum emitters is in-plane orientated. Additionally, we resolve the far-field emission pattern spectrally through back focal plane spectroscopy. The novel method allows us to also study emission lines of low intensity.

[1] K. Barthelmi et al., in: Applied Physics Letters 117, 070501 (2020). [2] J. Klein et al., in: Nature Communications 10, 2755 (2019). [3] J. Klein and L. Sigl., in: ACS Photonics 8, 669-677 (2021). [4] K. Barthelmi et al., (2024).

HL 45.9 Thu 16:30 EW 203

**Optimization of Circular Bragg Grating Resonators for Quantum Dot Photonic Cluster State Sources in the Telecom C-Band** — •Yorick Reum, Jochen Kaupp, Simon Betzold, Felix Kohr, Tobias Huber-Loyola, Sven Höfling, and Andreas Pfenning — Technische Physik, Julius-Maximilians-Universität Würzburg, Germany

A major technological bottleneck for the realization of measurement-based optical quantum computing is the production of strings of highly-entangled photons, *photonic cluster states*. Semiconductor quantum dots (QDs) were shown to be promising candidates for cluster state sources, but spin-decoherence and non-negligible excitonic lifetimes currently limit fidelity and length of the emitted states [1]. This challenge can be tackled by embedding the QD into a cavity with high Purcell enhancement, inducing faster recombination times. We show Purcell-enhanced single-photon emission in the *telecom C-band* from InAs quantum dots inside *circular Bragg grating ("bullseye")* cavities, with excitonic decay times of down to $\tau = (180 \pm 3)$ ps, corresponding to a Purcell factor of $F_P = (6.7 \pm 0.6)$ [2]. To further optimize these resonators, we develop *best-fitting cavities* with 3D finite-difference time-domain simulations and discuss novel strategies for *post-fabrication tuning* via atomic layer deposition.

[1] Cogan, D., et al., Deterministic generation of indistinguishable photons in a cluster state. Nat. Photon. 17, 324-329 (2023).
[2] Kaupp, J., et al., Purcell-Enhanced Single-Photon Emission in the Telecom C-Band. Adv Quantum Technol. 2023, 2300242.

# HL 46: Transport properties II

Time: Thursday 15:00–17:00 Location: ER 325

HL 46.1 Thu 15:00 ER 325

**Monitoring Cation Exchange in Individual Semiconductor Nanowires via Transistor Characterization** — •Daniel Lengle[1,2], Maximilian Schwarz[1], Alf Mews[1,2], and August Dorn[3] — [1]Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany — [2]The Hamburg Center for Ultrafast Imaging, 22761 Hamburg, Germany — [3]Innovationszentrum Niedersachsen, 30159 Hannover, Germany

The properties of nanostructures are largely determined by their material composition and their geometry. Chemical cation-exchange reactions allow for a controlled change of the elemental composition within a nanostructure while its geometry is preserved. However, controlling the exchange at the single particle level is challenging. Here, we investigate the successive cation-exchange with silver on individual semiconducting nanowires. For this purpose, nanowire field-effect transistors are fabricated via optical lithography. Then the cation exchange is performed by submerging the device in a silver-nitrate solution. By precisely timing the duration in the solution, the reaction progress and thus the exchange degree can be controlled. Transport measurements reveal a change in conductivity, charge carrier concentration, and mobility with progressing cation exchange. The approach presented here shows an efficient way to monitor the transport properties of individual nanostructures with a minimum of interference in the reaction. Nanowires with carefully adjusted elemental composition, and thus adjusted optoelectronic properties, could find a way into electrical devices such as sensors, transistors or batteries.

HL 46.2 Thu 15:15 ER 325

**Direct Observation of Hole Drift and Diffusion in Contacted Nanowires Under Local Illumination** — •Moritz Wehrmeister, Daniel Lengle, Carlo Höhmann, Christian Strelow, Alf Mews, and Tobias Kipp — Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany

Kelvin probe force microscopy (KPFM) is a method for measuring the surface potential. Being based on atomic force microscopy, KPFM enables investigating nanostructures, such as nanowires and nanosheets. Combining optical, electrical, and KPFM measurements in one setup enables advanced investigations of the charge-carrier separation in these materials and the properties of semiconductor-metal interfaces. We investigate individual electrically contacted CdS nanowires, by combining scanning photocurrent mapping (SPCM) and KPFM. The charge-carrier mobility information of SPCM extended by KPFM maps gives a more complete picture of the path and hurdles, the charge carriers take inside the nanodevice in operando. We show that upon local optical excitation, differences in charge-carrier mobilities of electrons and holes lead to an imbalance in the surface potential. At the point of illumination, positive charges accumulate, due to their lower mobility. KPFM reveals this imbalance and how it influences the potential drop along the biased CdS nanowire. Furthermore, performing KPFM while optically exciting the probed sample position monitors the excess of positive charge carriers for each position of the illuminated nanowire. A decrease of this excess shows how holes drift and diffuse into the contacts, where they contribute to the measured photocurrent.

HL 46.3 Thu 15:30 ER 325

**Simulation of Charge-Carrier Transport in Cadmium Sulfide Nanowires** — •Carlo Höhmann, Moritz Wehrmeister, Daniel Lengle, Alf Mews, and Tobias Kipp — Physikalische Chemie, Hamburg, Deutschland

Theoretical simulations form the backbone of experiments and help to confirm physical models, find material properties, and also provide more detail in results such as spatial resolution. Here we report on a numerical finite element simulation of single electrically contacted cadmium sulphide (CdS) nanowires using COMSOL Multiphysics software. The focus of the simulation is on the surface potential, the band alignment and the current-voltage behavior. The results are compared with experimental results obtained by local photocurrent microscopy and Kelvin probe force microscopy on single wet-chemically synthesized CdS nanowires. This comparison gives us a better understanding of the underlying physics and provides material parameters that are difficult to obtain by experiments alone.

We show that simulations based on the drift-diffusion approach including trap-assisted charge-carrier recombination at the surface, local photo excitation and ohmic metal contacts on the surface, is able to provide comparable results and new insights, for example, into the type of recombination or the exact location of the electrons and holes. We can also see how the system behaves under extreme conditions, such as high applied voltages or temperatures.

HL 46.4 Thu 15:45 ER 325

**Counter-Ion Size Effect on the Thermoelectric Properties of Doped Carbon Nanotubes Network** — •Aditya Dash[1], Angus Hawkey[2], Dorothea Scheunemann[1], Jana Zaumseil[2], and Martijn Kemerink[1] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Institute for Physical Chemistry, Universität Heidelberg, D-69120 Heidelberg, Germany

Doping is a proven technique to improve the thermoelectric properties of semiconducting single-walled carbon nanotube networks, which are promising for the conversion of waste heat to electricity. For this, understanding the counter-ion size effect is crucial, as Coulombic interactions between the ions and the free charge carriers cause scattering and trapping. Here, we propose a random resistor network model that accounts for the formation of Coulombic traps at low doping levels, and the formation of an impurity band at high doping levels. As such, it accounts for the increasing overlap of the Coulombic potentials due to dopant ions. The model semi-quantitatively reproduces our experiments that demonstrate that larger counter-ions enhance conductivity and maximize the power factor before a saturation sets in. Moreover, the conductivity dependence on ionic size is stronger at low temperatures. Overall, the employed model may guide the counter-ion selection to improve thermoelectric efficiency, depending on the interplay between the achievable doping level, ion size and the energetic disorder in the network.

**15 min. break**

HL 46.5 Thu 16:15 ER 325

**Universal Theory of Hall Transport in Organic Semiconductors** — •Michel Panhans and Frank Ortmann — TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany

The investigation of Hall transport is a key experimental method to understand transport mechanisms in organic semiconductors (OSCs). Despite many experimental observations of the Hall effect in OSCs, theoretical descriptions usually fail to understand these experiments.

This lack in the theoretical description motivated our recent study, where we develop a universal theory to understand the Hall effect in OSCs and beyond. Our new approach embeds previous theoretical descriptions covering different aspects of Hall transport ranging from semi-classical band-transport approaches, via topological descriptions utilizing geometrical concepts such as the Berry curvature to disorder driven transport scenarios.

Using rubrene as a showcase, we discuss the range of validity of different Hall-transport regimes and finally compare our results for the temperature-dependent Hall mobility to the experiment. The determination of the Hall mobility allows us to quantify the number of charge carriers that are responsive to the magnetic field. These results can be used to classify the charge transport in rubrene in terms of band-like and hopping transport at different temperatures.

HL 46.6 Thu 16:30 ER 325

**Hall field-induced resistance oscillations in two-dimensional Lorentz gases** — •Frederik Bartels, Johannes Strobel, Mihai Cerchez, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Two-dimensional electronic systems in non-equilibrium exhibit some exciting phenomena. One phenomenon are Hall field-induced resistance oscillations (HIROs), which can be recognized in the magnetoresistance of a highly mobile sample. Applying a direct current (x-direction) generates a tilt of the Landau levels due to the additional Hall field (y-direction). Tunneling to a higher Landau level is therefore possible, whereby the maximum probability depends on the shift in the y-direction. From theoretical considerations, a HIRO maximum arises

due to backscattering, because this leads to the maximum shift (by $2R_c$) in the y-direction for a single scattering event. We have investigated HIROs as a function of the obstacle density in two-dimensional Lorentz gases. A monotonous increase of the HIRO period with increasing density of the designed obstacles is observed. At large current densities, the HIROs deviate even qualitatively from the theoretical expectations. In addition, we determined the quantum scattering time $\tau_q$ and the backscattering time $\tau_\pi$ using the HIROs. The quantum scattering times from the HIROs are significantly larger than the quantum scattering time that can be determined from the Shubnikov-de Haas oscillations in the equilibrium.

HL 46.7 Thu 16:45 ER 325

**Identifying different electronic transport mechanisms in nanoporous inorganic C12A7 using Hall measurements and electron paramagnetic resonance spectroscopy** — •Julius K. Dinter[1], Jurek Lange[1,2], Detlev M. Hofmann[1,2], J. Fabián Plaza Fernández[3], Angel Post[3], Sangam Chatterjee[1,2], Matthias T. Elm[1,2,4], and Peter J. Klar[1,2] — [1]Center for Materials Research, Justus-Liebig University, Heinrich-Buff-Ring 16, D-35392, Giessen, Germany — [2]Institute of Experimental Physics I, Justus-Liebig University, Heinrich-Buff-Ring 16, D-35392, Giessen, Germany — [3]Advanced Thermal Devices, Calle Villaconejos, 4, E-28925, Alcorcón, Spain — [4]Institute of Physical Chemistry, Justus-Liebig University, Heinrich-Buff-Ring 17, D-35392, Giessen, Germany

$[Ca_{24}Al_{28}O_{64}]^{4+}(2O^{2-})$ is a nanoporous compound, whose properties are strongly determined by its degree of reduction. It consists of a positively charged cage and additional oxygen ions $O^{2-}$, which ensure charge neutrality and can move almost freely between them. A transition from insulating behavior to metallic behavior occurs when replacing the $O^{2-}$ ions in the cages by electrons, finally generating the electride $[Ca_{24}Al_{28}O_{64}]^{4+}$. However, a complete understanding of the charge transport mechanisms of the system and their variation with the degree of reduction is far from complete. Here, we present the characterization of a series of $[Ca_{24}Al_{28}O_{64}]^{4+}(2O^{2-})_{(1-x)}(4e^-)_x$ with different $x$ using Hall-measurements and electron paramagnetic resonance spectroscopy in a high temperature range. Three different transport mechanisms are identified which dominate at different temperatures.

## HL 47: 2D Materials: Heterostuctures

Time: Thursday 15:00–17:00 Location: EW 201

HL 47.1 Thu 15:00 EW 201

**Controlled Encapsulation of Monolayer $MoS_2$ with Ultrathin Aluminum Oxide for Tunnel Contacts** — •Sergej Levashov, Chenjiang Qian, Theresa Grünleitner, Jon J. Finley, Alex Henning, and Ian D. Sharp — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München

Two-dimensional (2D) semiconductors have unique optoelectronic properties that provide the opportunity to overcome current scaling and performance limits of semiconductor devices. Harnessing the full potential of 2D materials requires their seamless integration with bulk materials, which is challenging for mono- and few-layer 2D materials since the deposition process may introduce defects, thereby impeding interfacial charge transport. Here, we use low-temperature atomic layer deposition (ALD) to encapsulate monolayer $MoS_2$ with a van der Waals bonded and ultrathin aluminium oxide ($AlO_x$) layer. The weakly bonded 18 Å thin $AlO_x$ coating introduces additional charge carriers ($\sim 4\times10^{12}$ $cm^{-2}$) while it also protects monolayer $MoS_2$ from defect creation during metallization. Moreover, an $AlO_x$ thickness dependent study revealed an interface-dominated change in excitonic features. Fabricated field-effect transistors (FETs) show an additional charge transfer doping of up to $\sim 8.5\times10^{12} cm^{-2}$ due to trap state relaxation after inert gas annealing and, more importantly, a five-fold reduction in the contact resistance for $MoS_2$ FETs contacted with an $AlO_x$ interlayer. Overall, this work shows the beneficial effect of the ALD $AlO_x$ adlayer for improving 2D device contacts and provides a scalable route to the damage-free integration of 2D semiconductors.

HL 47.2 Thu 15:15 EW 201

**Investigation of electric contacts to 2D semiconductors for optoelectronic and solar energy conversion application** — •Ariane Ufer[1], Hendrik Lambers[1], Benjamin Mayer[1], Emeline Nysten[1], Hubert Krenner[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

Two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDCs) such as molybdenum disulfide ($MoS_2$) are of great interest as they exhibit outstanding optoelectronic properties. Due to the highly efficient exciton dominated light-matter interaction, TMDC mono- and multilayers are promising materials for optoelectronic and solar energy conversion applications with the potential to provide lightweight, flexible, versatile, and robust devices. For these applications the contacts between the semiconducting TMDC and the conducting material play a significant role, whereby the major challenge for high power conversion efficiencies (PCE) is the separation and collection of charge carriers. We fabricate semiconductor-metal junctions by transferring $MoS_2$ mono- and multilayers by dry viscoelastic stamping techniques on top of various nanofabricated metallic contact pads. The samples are characterized via photoluminescence (PL) and Raman spectroscopy. Furthermore, we study the charge transfer across the 2D semiconductor-metal heterojunction using local laser beam induced current measurements.

HL 47.3 Thu 15:30 EW 201

**Broadband Dielectric Mirrors and Microcavity Configurations for Multimode Coupling with Excitons in TMDC Heterostructures.** — •Chirag Palekar[1], Bárbara Rosa[1], Niels Heermeier[1], Ching-Wen Shih[1], Imad Limame[1], Aris Kaulas-Simos[1], Arash Rahimi-Iman[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

We introduce chirped distributed Bragg reflectors with a broad stopband (>600 nm), spanning visible to near-infrared wavelengths. Our microcavity configurations employ broadband chirped DBRs which consist SiO2 and Si3N4 layers, demonstrating energetically separated cavity resonances. These modes are utilized to investigate the light-matter interactions with intra- and inter-layer excitons of transition metal dichalcogenide bilayer heterostructures (TMDC HSs). Additionally, our chirped microcavity systems shows cavity-coupled emission of energetically separated intra and interlayer excitons in a WSe2/MoSe2 heterostructure. The microcavity, combined with TMDC HSs, holds promise for studying moiré physics and advancing light-matter interactions in TMDC-based devices. Overall, our approach provides a versatile tool for future studies of spectrally distant and confined excitons in any active medium which paves the way for various applications by enabling precise control and manipulation of excitonic interactions utilizing multimode resonance light-matter interaction.

HL 47.4 Thu 15:45 EW 201

**Distance dependence of the energy transfer mechanism in $WS_2$-graphene heterostructures** — •David Tebbe[1], Marc Schütte[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], Bernd Beschoten[1], and Lutz Waldecker[1] — [1]2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany — [2]Research Center for Functional Materials, National Institute for Materials Science, Japan — [3]International Center for Materials Nanoarchitectonics, Japan

We investigate the mechanism of energy transfer in heterostructures of the two-dimensional semiconductor $WS_2$ and graphene with variable interlayer distances achieved through spacer layers of hexagonal boron nitride (hBN). Our analysis of the emission and absorption line widths reveals that the energy transfer is dominated by states outside the light cone, indicating a Förster transfer process. The dependence of luminescence intensity on interlayer distances above 1 nm can be quantitatively reproduced using recently calculated values of the Förster transfer rates of thermalized charge carriers and a constant radiative rate. However, at smaller interlayer distances, the experimentally observed transfer rates exceed the predictions and depend on excess energy and

excitation density. We conclude that at these distances, the transfer is driven by non-thermalized charge carrier distributions, as the transfer probability of the Förster mechanism depends on the momentum of electron-hole pairs.

HL 47.5 Thu 16:00 EW 201

**Evaluation of Disorder in Graphene Layers via Raman Spectroscopy for Enhanced Device Fabrication in Microelectronics** — •Farnaz Majnoon[1], Rasuole Lukose[1], Daniele Capista[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP-Leibniz Institute für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

Graphene, a two-dimensional (2D) material, has emerged as a promising candidate for next-generation microelectronics owing to its exceptional electrical, mechanical, and thermal properties. In this study, we employ Raman spectroscopy as a powerful tool to probe the distinctiveness of graphene. The investigation focuses on elucidating the relationship between Raman spectral features and the quality of graphene layers, offering insights into its suitability for industrial microelectronics applications. Our analysis delves into the vibrational modes exhibited by graphene, exploring the effects of layer thickness, defects, and doping on the Raman spectra. The distinct G, D, and 2D bands provide crucial information regarding the structural integrity and quality of graphene, crucial parameters in evaluating its viability for microelectronic devices. We examine the impact of various contact methods and materials on graphene, aiming to comprehend their role in introducing disorder. Through Raman spectroscopy, this study reveals changes in graphene's properties influenced by these factors. These insights are pivotal in identifying the origins and scale of disorder, essential for refining fabrication processes and to achieve superior performance.

HL 47.6 Thu 16:15 EW 201

**Effect of Energy Bands Overlap in the Interlayer Energy Transfer Processes in 2D Heterostructures** — •Arka Karmakar — University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Heterostructures (HSs) made by the monolayers (1Ls) of transition metal dichalcogenides (TMDs) have shown great promises in designing next-generation optoelectronic device applications. Interlayer charge (CT) and energy transfer (ET) processes are the main photocarrier relaxation pathways in the TMD HSs. CT processes mainly occur due to the energy level offset between the materials and can survive only up to a few nm. Whereas, the interlayer ET process mediated by the dipole-dipole coupling between the donor and acceptor materials, can survive up to several tens of nm. In this talk, I would like to present our recent studies to understand the effect of energy bands overlap in the ET process in TMD HSs. First, we showed that in the type-II HSs formed using the 1Ls of molybdenum diselenide (MoSe2) and rhenium disulfide (ReS2), an ET process dominates over the fast CT process, resulting 360% photoluminescence (PL) enhancement in the HS area. After completely blocking the CT process, this enhancement increased further up to more than 1 order of magnitude higher. Next, we showed that HS formed between the 1Ls of molybdenum disulfide (MoS2) and tungsten disulfide (WSe2), an unusual ET process occur from the lower bandgap WSe2 to higher bandgap MoS2 due to the resonant overlaps between the high-lying excitonic states. These works will help us to realize the complex ET processes in TMD HSs for better development of the TMD-based novel optoelectronic device applications.

HL 47.7 Thu 16:30 EW 201

**Fabrication and Characterization of van der Walls Layers with Improved Interfacial Quality** — •Laura Nicolette Schusser[1], Nihit Saigal[1], Hossein Ostovar[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]University of Münster, Germany — [2]University of Chemistry and Technology Prague,Czech Republic

The rich physical properties of two-dimensional materials, such as transition-metal dichalcogenides (TMDC) and related heterostructures have ushered in a new era of emergent phases and the development of devices [1,2]. Micromechanical exfoliation combined with the deterministic dry transfer of two-dimensional crystals represents a critical advancement in the fabrication of heterostructures through the controlled stacking of two-dimensional materials [2]. However, the presence of interfacial residuals and contaminants adversely affects the quality of heterostructures, consequently impacting the electrical and optical properties of the material. We established a fully automated setup for the dry transfer of two-dimensional materials inside a glovebox in a controlled environment. The quality of bulk crystals plays a crucial role in the fabrication of heterostructures. We utilize photoluminescence (PL) spectroscopy combined with Raman spectroscopy for the characterization of 2D layers exfoliated from differently grown TMDC crystals. [1] N. Saigal et. al., Arxiv Preprint, (2023). [2]Y. Lei et al., ACS Nanoscience Au2.6(2022)

HL 47.8 Thu 16:45 EW 201

**Light Sources with Bias Tunable Spectrum based on van der Waals Interface Transistors** — •Nicolas Ubrig[1], Hugo Henck[1], Diego Mauro[1], Ignacio Gutiérrez-Lezama[1], Luis Balicas[2], and Alberto Morpurgo[1] — [1]Department of Quantum Matter Physics, University of Geneva — [2]ational High Magnetic Field Laboratory, Tallahassee, FL 32310, USA

Light-emitting electronic devices are ubiquitous in key areas of current technology, such as data communications, solid-state lighting, displays, and optical interconnects. Controlling the spectrum of the emitted light electrically, by simply acting on the device bias conditions, is an important goal with potential technological repercussions. However, identifying a material platform enabling broad electrical tuning of the spectrum of electroluminescent devices is difficult. Here, we propose light-emitting field-effect transistors based on van der Waals interfaces of atomically thin semiconductors as a promising class of devices to achieve this goal. We demonstrate that large spectral changes in room-temperature electroluminescence can be controlled both at the device assembly stage –by suitably selecting the material forming the interfaces– and on-chip, by changing the bias to modify the device operation point. As the physical mechanism responsible for light emission is robust and does not depend on details of the interfaces, these structures are compatible with simple large areas device production methods.

# HL 48: Quantum Dots and Wires: Growth

Time: Thursday 15:00–16:30 Location: EW 202

HL 48.1 Thu 15:00 EW 202

**Doping of GaAs/AlGaAs core-shell nanowires by ion implantation** — •Yuxuan Sun[1,2], Donovan Hilliard[1,2], Emmanouil Dimakis[1], Shengqiang Zhou[1], Manfred Helm[1,2], and Slawomir Prucnal[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany; — [2]Technische Universität Dresden, 01062 Dresden, Germany

III-V semiconductor core-shell nanowires are promising for high electron mobility transistors and one-dimensional electron transport, which can be integrated on a nanoscale platform. Core-shell heterostructures are typically designed so that electrons are confined inside the thin core, which is surrounded by a relatively thick undoped shell with wider bandgap. This makes it challenging to form ohmic contacts for the measurement of the electrical properties of the core or the fabrication of devices. Here, we present the contact engineering to GaAs:Si/AlxGa1-xAs core-shell nanowires using selective area ion-implantation of Sulphur. The properly chosen energy of the ion-implantation and selective area implantation allow precise control of the carrier concentration just below the metal contact. Such an approach provides electrical connection to the core nanowire without degrading the crystal structure of the entire nanowire. For electrical activation of implanted impurities we have used ms-range Flash lamp annealing and rapid thermal annealing. Detailed structure, optical and electrical characterization of the nanowires will be presented.

HL 48.2 Thu 15:15 EW 202

**Influence of InAl deposition amount and annealing time on nanohole formation by local droplet etching on $In_{0.52}Al_{0.48}As$ layers** — •Dennis Deutsch[1], Christopher Buchholz[1], Viktoryia Zolatanosha[1,2], Klaus D. Jöns[1,2], and Dirk Reuter[1,2] — [1]Department of Physics, Paderborn University, Paderborn, Germany — [2]Institute for Photonic Quantum Systems (PhoQS), Paderborn University, Paderborn, Germany

Semiconductor quantum dots are excellent candidates for on-demand generation of entangled photon pairs. Especially $GaAs/Al_xGa_{1-x}As$ quantum dots grown via the local droplet etching approach have been proven to be very promising sources, due to their low strain and excellent in-plane symmetry. However, for the $GaAs/Al_xGa_{1-x}As$ system one is limited to photon emission around 780 nm and ideally photons would be generated in the optical C-band (1530 - 1565 nm) to utilize established fiber networks. One solution is to transfer the local droplet etching technique to the $InP/In_yAl_{1-y}As/In_xGa_{1-x}As$ system. In this contribution we report on the etching of nanoholes into $In_{0.52}Al_{0.48}As$ layers by depositing InAl droplets. We show how the amount of deposited material influences the size, shape and density of the drilled nanoholes. We further display the effect of varying the annealing time after the initial droplet droplet deposition step. Finally, we present that the filled nanoholes emit light when embedded in an $In_{0.52}Al_{0.48}As$ matrix and that we can create quantum dots that show emission up into the optical C-band.

HL 48.3 Thu 15:30 EW 202

**High-quality single InGaAs/GaAs quantum dots grown on a CMOS-compatible silicon substrate for quantum photonic applications** — •Imad Limame[1], Peter Ludewig[2], Ching-Wen Shih[1], Marcel Hohn[1], Chirag C. Palekar[1], Wolfgang Stolz[2], and Stephan Reitzenstein[1] — [1]ISSP, Technical Univ. of Berlin, DE — [2]NAsP III/V GmbH, Philipps-Univ. of Marburg, DE

Despite significant advances in silicon photonics employing classical light sources, advancements in silicon-compatible quantum photonics have been hindered by the challenge of achieving direct and high-quality growth of single quantum dots (QDs) on the silicon platform. While there have been advancements in post-growth QD integration on silicon, the intricacies of the process restrict scalability and cost-effectiveness. Silicon quantum photonics seeks to harness the unique properties of quantum systems-such as superposition, entanglement, and photon indistinguishability-to facilitate a cost-effective integration of cutting-edge silicon electronics and advanced quantum photonics.

We report on the direct growth of InGaAs QDs with excellent quantum optical properties on a CMOS-compatible silicon substrate [1]. The heteroepitaxy of GaAs heterostructures on silicon is accomplished through a GaP buffer layer. Under non-resonance excitation, we measure high multi-photon suppression of 0.037, and good photon indistinguishability of 0.66. Furthermore, we achieve an extraction efficiency of up to 18.35% for the as-grown QDs with a backside distributed Bragg mirror, showcasing the significant potential of the developed approach.

[1] Limame, I. et al., Preprint at arXiv:2311.14849 (2023)

HL 48.4 Thu 15:45 EW 202

**Droplet-etched GaAs quantum dots integrated in AlGaAs photonic circuits as a source of highly indistinguishable photons** — •Ulrich Pfister[1], Florian Hornung[1], Stephanie Bauer[1], Dee Rocking Cyrlyson's[2], Ponraj Vijayan[1], Ailton J. Garcia Jr[2], Saimon Filipe Covre da Silva[2], Michael Jetter[1], Simone L. Portalupi[1], Armando Rastelli[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, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

Droplet-etched GaAs quantum dots (QDs) are a promising source of single and highly indistinguishable photons. Their optical properties like narrow wavelength distribution, short decay times, linewidths near to the Fourier limit and the resulting highly indistinguishable photons make them highly appealing for several quantum technologies [1]. We demonstrate the first integration of these QDs in photonic integrated circuits consisting of single-mode waveguides and multi-mode interference splitters [2].Under pulsed resonant excitation we achieved high single photon purities of up to $1 - g^{(2)}(0) = 0.929 \pm 0.009$ and two-photon interference visibilities of consecutively emitted photons of $0.939 \pm 0.009$.

[1] S. F. C. da Silva, *et al.*, Applied Physics Letters, **119**,12 (2021)
[2] Florian Hornung, *et al.*, arXiv:2310.11899 (2023)

HL 48.5 Thu 16:00 EW 202

**Separating nucleation and growth during the synthesis of perovskite quantum dots** — •David Ederle, Jochen Feldmann, and Quinten A. Akkerman — Chair for Photonics and Optoelectronics, Department of Physics, Nano-Institute Munich, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

Due to their unique optoelectronic properties, colloidal lead halide perovskite quantum dots (LHP QDs) have received much attention in recent years.[1] With a near-unity photoluminescence (PL) quantum yield and highly tuneable PL with a narrow emission, this group of materials is of interest for research and applications such as light-emitting devices and photovoltaics. As the properties of the QDs strongly depend on their size and shape, complete control over their synthesis is crucial. Nonetheless, the search for suitable reaction conditions to synthesize LHP QDs of a certain size remains challenging.

Here, we present a synthesis protocol which allows to temporally separate the nucleation and growth, facilitating the synthesis of monodisperse QDs of a specific size.[2] In this process, in-situ absorption spectroscopy provides a suitable tool for live monitoring the kinetics of the nucleation and growth. This allows us to gain a better understanding of what drives the challenging synthesis of LHP QDs and how to control it.

[1] A. Dey et al., *ACS Nano* **15**, 10775-10981 (2021).
[2] Q. A. Akkerman et al., *Science* **377**, 1406-1412 (2022).

HL 48.6 Thu 16:15 EW 202

**Wafer-Scale Emission Energy Modulation of Indium Flushed Quantum Dots** — •Nikolai Spitzer, Nikolai Bart, Hans-Georg Babin, Marcel Schmidt, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum, Germany

We explore a novel approach for fine-tuning the emission wavelength of quantum dots (QDs) by building upon the indium flush growth method: Submonolayer variations in the capping thickness reveal a non-monotonic progression, where the emission energy can decrease even though the capping thickness decreases. Indium flush, a well-known technique for inducing blue shifts in quantum dot emissions, involves the partial capping of QDs with GaAs followed by a temperature ramp-up. However, our findings reveal that the capping layer

roughness, stemming from fractional monolayers during overgrowth, plays a pivotal role in modulating the emission energy of these QDs. We propose increased indium interdiffusion between the QDs and the surrounding GaAs capping layer for a rough surface surrounding the QD as the driving mechanism. This interdiffusion alters the indium content within the QDs, resulting in an additional emission energy shift, counterintuitive to the capping layers thickness increase. We utilize photoluminescence spectroscopy to generate wafer maps depicting the emission spectrum of the QDs. Using thickness gradients, we produce systematic variations in the capping layer thickness on 3-inch wafers, resulting in modulations of the emission energy of up to 26 meV.

## HL 49: Semiconductor Lasers II

Time: Thursday 15:00–16:45 Location: EW 561

**Invited Talk** HL 49.1 Thu 15:00 EW 561

**Dynamical laser properties of tunnel-injection devices.** — •Michael Lorke[1], Frank Jahnke[1], Gadi Eisenstein[2], and Johann-Peter Reithmeier[3] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]Electrical Engineering Department and Russel Berrie Nanotechnology Institute, Technion, Haifa, Israel — [3]Technische Physik, Institute of Nanostructure Technologies and Analytics, Kassel

Tunnel injection lasers are an appealing concept for the next generation of semiconductor lasers, as they promise improved modulation rates and better temperature stability. Moreover, they eliminate a major detrimental effect of quantum dot lasers, which is the gain nonlinearity caused by hot carriers. The introduction of a tunnel barrier for controlling the coupling of quantum dots (QDs) to an injector quantum well (QW) introduces significant design changes in comparison to conventional QD or QW lasers. As a result, nanoscale physics and quantum mechanical interaction processes take a more important role in the device properties. This poses new challenges to our theoretical understanding and increases the need for applying microscopic models. We present a theoretical study of dynamical laser properties inclusing the transport within the device and show the impact of alignment between the injector quantum well and the QDs on the laser switch-on process and modulation properties. These are important for the use of these laser systems in novel telecommunication applications.

HL 49.2 Thu 15:30 EW 561

**High-speed low-noise wafer-fused MBE-grown 1550 nm VCSELs** — •Sicong Tian[1,2], Georgiy Sapunov[1], Sergei Blokhin[3], Andrey Babichev[4], Innokenty Novikov[4], Anton Egorov[5], Leonid Karachinsky[4], and Dieter Bimberg[1,2] — [1]imberg Chinese-German Center for Green Photonics, Changchun Institute of Optics, Fine Mechanics, and Physics, Chinese Academy of Sciences, Changchun 130033, PR China — [2]Center of Nanophotonics, Institute of Solid State Physics, Technische Universität Berlin, Berlin D-10632, Federal Republic of Germany — [3]Saint Petersburg, Russia — [4]Saint Petersburg, Russia — [5]Saint Petersburg, Russia

High-power low-noise wafer-fused MBE-grown 1550 nm VCSELs with an InP-based optical cavity with InGaAs QWs and a composite InAlGaAs 6 $\mu$m BTJ and AlGaAs/GaAs distributed Bragg reflectors are fabricated. The VCSELs demonstrate 5 mW single-mode continuous-wave output optical power at 20 °C and 1 mW at 70 °C. Over 13 GHz 3dB modulation bandwidth is obtained at 20 °C. NRZ data rate of 37 Gbps under BTB condition is shown. A preliminary study shows RIN $<$ -156 dB/Hz and a data rate $>$ 50 Gbit/s at a 500 m distance under PAM4 modulation.

HL 49.3 Thu 15:45 EW 561

**High-beta quantum dot micropillar lasers operating at room temperature** — •Sarthak Tripathi, Floriana Laudani, Kartik Gaur, Imad Limame, Ching-Wen Shih, Sven Rodt, and Stephan Reitzenstein — Inst. for Solid State Phys., Technical Univ. of Berlin, Germany

Room temperature micropillar lasing has attracted significant attention due to its potential applications in integrated photonics, optoelectronics, and neuromorphic computing. In this study, we present the fabrication and characterization of micropillar lasers showing a room-temperature emission wavelength around 960 nm. The epitaxially grown structure consists of a central one-lambda GaAs cavity with integrated InGaAs quantum dots (QDs), which is sandwiched between bottom and top distributed Bragg reflector (DBR) pair. Based on such planar microcavity structures high-Q micropillar cavities are fabricated using electron beam lithography and dry etching techniques, resulting in uniform pillar dimensions. Multiple layers of high-density InGaAs QDs are stacked in the active region in order to maximize the modal gain of the micropillar resonators for room-temperature operation. The density of dislocations and point defects in QDs heterostructures is strongly reduced by post-growth annealing which enables us to blue shift in wavelength without forfeiting their crystalline quality. Numerical simulations are carried out to optimize the fabrication parameters and subsequently validate the optical properties. Moreover, photoluminescence studies are conducted to evaluate the optical and laser properties of micropillar cavities.

HL 49.4 Thu 16:00 EW 561

**Radially doped InGaAs-GaAs(Sb)/AlGaAs multi-quantum well nanowire laser structures on silicon** — •Sebastian Werner, Tobias Schreitmüller, Hyowon Jeong, Paul Schmiedeke, Jonathan Finley, and Gregor Koblmüller — Walter Schottky Institute, Technical University of Munich, 85748 Garching, Germany

The ability to integrate III-V semiconductor nanowires (NW) on silicon (Si) platform opens many perspectives for advanced optoelectronic and photonic device applications on-chip. However, for energy-efficient device performance, as in III-V NW-solar cells, light emitting diodes (LEDs) or laser diodes, the design of accurately doped heterostructures and the optically active region is very crucial. In this contribution, we present our developments of radially doped n-i-p core-multishell NW hetero-structures monolithically integrated on the n-Si (111) platform for compact NW laser diode devices in the near-infrared spectral range. The NW structure is designed to host n-type doped GaAs(Sb) cores, while the shell is composed of (In,Al)GaAs(Sb)-based heterojunctions that define intrinsic multi-quantum well (MQW) active and p-type doped regions. Under optical pumping schemes, we show that n-doped (Si-doped) GaAs(Sb) NWs show lasing characteristics, with a doping dependent lasing threshold $<$ 50 $\mu$J/cm$^2$. Extending these experiments to fully doped radial heterojunctions hosting seven coaxial InGaAs/GaAs MQWs, we further demonstrate low-threshold lasing of $<$ 43 $\mu$J/cm$^2$ (10K) and even up to $\sim$150K in an integrated vertical-cavity geometry on Si.

HL 49.5 Thu 16:15 EW 561

**Numerical investigation of the far-field behavior of VCSELs with monolithic high contrast gratings** — •Lilli Kuen[1,2], Mikołaj Janczak[3], Marcin Gebski[3], Tomasz Czyszanowski[3], Sven Burger[1,2], Stephan Reitzenstein[4], and Martin Hammerschmidt[1,2] — [1]Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany. — [2]JCMwave GmbH, Bolivarallee 22, 14050 Berlin, Germany. — [3]Institute of Physics, Lodz University of Technology, 93-005 Łódź, Poland. — [4]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany.

Vertical-cavity surface-emitting lasers (VCSELs) are widely used light sources, and their functional principle is well known. A novel approach to control the resonant wavelength and the polarisation state is to replace the upper DBR mirror with a line grating with finite size and high contrast material, a so-called monolithic high contrast grating (MHCG).

In this contribution, we investigate the far-field behavior of such structures with respect to the oxide aperture width, the size of the grating, and the number of grating periods. This enables a better understanding of the relation between oxide aperture width and the finite grating size on the most important properties of VCSELs with MHCG.

In our numerical study, we compute resonance modes, which are solutions to Maxwell's equations without sources. To this aim, we employ a finite-element method. The far-field pattern is obtained by using a near-field to far-field transformation.

HL 49.6 Thu 16:30 EW 561

**Gain characteristics of AlGaN quantum wells for UVC laser diodes application** — •Giulia Cardinali[1], Alexander Schulz[1], Sebastian Kölle[2], Friedhard Römer[2], Bernd Witzigmann[2], Norman Susilo[1], Daniel Hauer Vidal[1], Martin Guttmann[1], Tim Wernicke[1], and Michael Kneissl[1,3] — [1]Technische Universität Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]University of Erlangen-Nürnberg (FAU), Department of Electrical Engineering, Erlangen, Germany — [3]Ferdinand-Braun-Institut (FBH), Berlin, Germany

UVC laser diodes have small size, low cost and high output power, providing a viable alternative to 266 nm frequency-quadrupled solid-state lasers. Thick AlGaN single quantum wells (SQW) with large confinement factors are advantageous for UVC devices, and can achieve relatively low thresholds despite the large polarization fields. In this study, AlGaN UVC optically pumped lasers with a SQW active region with thickness between 3 nm and 12 nm were fabricated with m-plane resonators and cavity lengths between 600 $\mu$m and 1400 $\mu$m. The threshold power density decreases with increasing QW width, with the lowest value of 1.3 MW/cm$^2$ for a 9 nm SQW laser. All the samples exhibited positive gain for all QW widths, with the highest differential gain for the 9 nm SQW, in correspondence of the minimum of the threshold. The high gain and low threshold of thick AlGaN QWs are explained by k·p simulations, showing a large electron-hole wavefunction overlap at high carrier density in thick wells, where a high contribution to the gain also comes from excited state transitions.

## HL 50: Members' Assembly

Organized by Axel Lorke, Stephan Reitzenstein, and Alexander Holleitner

Time: Thursday 17:00–18:30 Location: EW 202

**All members of the Semiconductor Physics Division are invited to participate.**

## HL 51: Functional Semiconductors for Renewable Energy Solutions II

Time: Friday 9:30–11:00 Location: ER 325

HL 51.1 Fri 9:30 ER 325

**Investigation of a LID defect energy barrier using a P-line appearing in indium-doped silicon PL spectra** — •Katharina Peh[1], Dominik Bratek[1], Kevin Lauer[1,2], Robin Lars Benedikt Müller[1], Dirk Schulze[1], Aaron Flöttotto[1] und Stefan Krischok[1] — [1]TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

With the help of low-temperature photoluminescence (LTPL) it is possible to find photoluminescence (PL) lines that originate from defects. These PL lines can indicate not only the species, but also the density of one specific defect configuration. In indium-doped silicon, the P-line at 1.118 eV is used to investigate light-induced degradation (LID). [1,2] With illumination and annealing treatments, we are now able to reproducibly influence the intensity of the P-line, and thus identify the P-line as an intermediate state. It will be discussed within the $A_{Si}$-$Si_i$ defect model. [3] Both Czochralski (CZ) and float zone (FZ) silicon wafers were examined and their behaviour compared. For the first energy barrier in annealing treatments of the LID defect, we obtain values between $E_{FZ}$=0.5±0.09 to $E_{CZ}$=0.84±0.22 eV. [4] [1] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5(1), 017101 (2015). [2]C. Möller, and K. Lauer, Physica Status Solidi (RRL) - Rapid Research Letters 7(7), 461-464 (2013). [3]K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, Physica Status Solidi (a) 219(19), 2200099 (2022). [4]D. Bratek, Master thesis (2023).

HL 51.2 Fri 9:45 ER 325

**The influence of structural dynamics on the macroscopic properties of the solar harvesting nitride CuTaN2** — •Franziska S. Hegner[1], Adi Cohen[2], Stefan S. Rudel[3], Silva Kronawitter[1], Manuel Grumet[1], Xiangzhou Zhu[1], Roman Korobko[2], Lothar Houben[2], Chang-Ming Jiang[1], Wolfgang Schnick[3], Gregor Kieslich[1], Omer Yaffe[2], Ian D. Sharp[1], and David A. Egger[1] — [1]TU Munich, Germany — [2]Weizmann Institute of Science, Israel — [3]LMU Munich, Germany

Ternary nitrides are an emerging class of materials that show large potential for solar energy conversion because of their favourable light absorption and carrier transport properties. Yet, they are relatively unexplored due to their metastability and the comparative difficulty of their synthesis. Here, we studied the representative copper tantalum nitride, CuTaN2, a particularly promising visible light absorbing semiconductor, using a combination of theoretical and experimental methods. Harmonic phonon calculations and finite-temperature Raman scattering experiments show that its structural dynamics display highly anharmonic character. We first elucidated the microscopic aspects of the atomic motions with ab initio Molecular Dynamics and then investigated their impact on their macroscopic characteristics. The latter are strongly influenced by the anharmonic nuclear motions, leading to negative thermal expansion and, especially important, a significant increase of the fundamental bandgap. This highlights that structural dynamics play a crucial role for the functional properties of energy materials.

HL 51.3 Fri 10:00 ER 325

**Luminescence study of light induced degradation in thallium implanted silicon** — •Robin Lars Benedikt Müller[1], Kevin Lauer[1,2], Katharina Peh[1], Zia Ul-Islam[1], Dirk Schulze[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Light-induced degradation (LID) designates the loss of efficiency of doped silicon-based devices such as solar cells and detectors. Despite extensive research into this phenomenon in recent decades, the recombination-active defect responsible for degradation remains unidentified until today. Thereby a variety of dopants were examined, besides boron and copper, indium doped silicon was investigated. A potential explanation for LID in Si:In is the so-called ASi-Sii defect, whose possible defect configurations manifests itself by the appearance of the P-line in the spectrum of low-temperature photoluminescence (LTPL)[1]. Besides this P-line, the spectra of thallium-doped silicon reveal a so-called A-line, whereby this unusual luminescence system is based on a defect which is present in two different configurations[2]. After the first demonstration of LID in Si:Tl, we investigated differently doped samples with regard to the behaviour of these spectral elements under the influence of the LID cycle.[1] K.Lauer, C.Moeller, D.Schulze, and C. Ahrens. AIP Advances, 5(1):017101, 01 2015; [2] H. Conzelmann, A. Hangleiter, and J. Weber. physica status solidi (b), 133(2):655*668, 1986.

HL 51.4 Fri 10:15 ER 325

**Water interaction in dependence of AlInP(100) surface reconstruction studied by in-situ RAS and XPS** — •Mohammad Amin Zare Pour, Sahar Shekarabi, Agnieszka Paszuk, and Thomas Hannappel — Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau

n-AlInP(100) is commonly used for a selective transport of electrons in so-called window layers in high-efficiency III-V multijunction solar or photoelectrochemical (PEC) cells. A fundamental understanding of water interaction with the window layer is crucial for PEC applications as well as for atomic layer deposition of passivation layers such as TiO2. In this study, we investigate reaction mechanisms of water with well-defined surfaces using X-ray photoelectron spectroscopy (XPS) and in-situ reflection anisotropy spectroscopy (RAS). As pre-

pared phosphorous rich and indium rich terminated n-AlInP(100) prepared by metalorganic chemical vapour deposition were exposed to water at room temperature and 10-5 mbar in an ultra-high vacuum chamber. In this work, exposure dosage was measured in langmuir (L) units, where 1 L = 1 Torr x 1s. Even after 75 kL of water exposure, the core-levels of P-rich AlInP do not exhibit any shift or significant changes in the line shape of the spectra. In contrast, In-rich AlInP is more likely to react with water molecules, and the RAS signal clearly changes after only 20 kL. The XPS results indicate that In-In bonds on In-rich surfaces are active sites, while neither P-P bonds nor III-P bonds on P-rich surfaces interact with water.

HL 51.5 Fri 10:30 ER 325

**Emerging oxynitride photoelectrodes for stable and efficient energy conversion** — •Tobias Haubold — Walter-Schottky-Institute, Technische Universität München, Germany

Photoelectrochemical solar water splitting represents a promising approach for the direct conversion of visible light into chemical fuels. To overcome the efficiency and stability limitations of pure oxide and nitride photosystems, respectively, high-throughput computational screening has identified oxynitrides as an interesting material space that offers narrower bandgaps and improved charge carrier mobility. While several studies have reported the synthesis of oxynitrides and demonstrated their application for photoelectrochemical energy conversion, controlled synthesis routes for high-quality materials and a fundamental understanding of semiconductor and defect-related properties are still lacking. Here, we leverage reactive magnetron sputtering and subsequent annealing as a controllable synthesis platform to deposit tantalum oxynitride thin films with controlled structure, chemical composition, and optoelectronic quality. By variation of the N2-O2 process gas mixture, we were able to systematically study the impact of anion non-stoichiometry on optical properties and photoelectrochemical performance. The gained insights will reveal the impact of electronically active oxygen- and nitrogen-related defect states within the bandgap on the semiconductor properties of oxynitrides.

HL 51.6 Fri 10:45 ER 325

**Engineering interfaces for efficient and stable photoelectrochemical energy conversion** — •Julian Müller[1,2], Matthias Kuhl[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

For photoelectrochemical (PEC) energy conversion, transition metal nitrides emerged recently as a promising alternative to commonly studied metal oxides. Among others, tantalum nitride (Ta3N5) is highly interesting due to its bandgap of 2.1 eV, suitable band alignment for water splitting, and theoretical photocurrent density of 12.9 mA/cm2. However, Ta3N5 rapidly degrades under operation conditions due to self-oxidative decomposition in aqueous electrolytes. Here, we interfaced Ta3N5 photoanodes with cobalt oxide (CoOx) surface layers to overcome the current stability limitations. Specifically, we leveraged plasma-enhanced atomic layer deposition (PE-ALD) to deposit stable, conformal, and ultra-thin protection layers which are simultaneously robust and electrochemically active. To engineer efficient interfaces between photoelectrode and protection layer, we developed one- and two-step annealing processes in different gas atmospheres and correlated the change in interface properties to their PEC characteristics. Overall, this study highlights the beneficial role of the protection layer on the photoelectrode stability, but also emphasizes the dominating role of interface properties on the efficiency and the need for controlled interface engineering.

## HL 52: Nitrides: Devices

Time: Friday 9:30–12:00 Location: EW 015

HL 52.1 Fri 9:30 EW 015

**Heterostructure optimization of far-ultraviolet C light emitting diodes for improved efficiency and lifetime** — •Tim Kolbe, Sylvia Hagedorn, Jens Rass, Hyun Kyong Cho, Jan Ruschel, Sven Einfeldt, and Markus Weyers — Ferdinand-Braun-Institut (FBH), Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

The development of AlGaN-based light emitting diodes (LEDs) with emission wavelength in the far-ultraviolet-C (far-UVC) spectral region ($<$ 240 nm) is driven by various applications like monitoring of gas concentrations (e.g. NO, NH3), the measurement of nitrates in water, or skin-friendly UVC-antisepsis. Although these LEDs have been improved over the recent years, the maximum emission power of the devices and their lifetimes are still low compared to UV LEDs in the longer wavelength range. In this presentation, an overview of our far-UVC LED development will be given. The influence of the heterostructure design and optimization of the epitaxial growth processes on voltage, emission power, and reliability of far-UVC LEDs will be discussed. Among other things, it will be shown how the design of the active region (e.g. quantum well numbers and quantum well barrier height) influences the voltage, optical power, and lifetime of the LEDs. Based on these optimizations, 233 nm LEDs with a maximum peak external quantum efficiency (EQE) of 1.13 % (wall plug efficiency of 0.82 %), an emission power of 9.7 mW and an operation voltage of 7.9 V at 200 mA were realized.

HL 52.2 Fri 9:45 EW 015

**Hole transport in AlGaN-based far-UVC LEDs with multiple quantum wells** — •Franz Biebler[1], Marcel Schilling[1], Jakob Höpfner[1], Massimo Grigoletto[2], Tim Wernicke[1], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut gGmbH, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

Understanding the hole transport in AlGaN-based far-UVC LEDs with wavelengths below 240 nm is crucial for improving the efficiency of these devices. In order to obtain an insight into this topic far-UVC LEDs with mixed wavelength AlGaN multiple quantum wells (MQW) were grown by metal organic vapor phase epitaxy (MOVPE), consisting of multiple QWs emitting at 233 nm and a single QW emitting at 250 nm. When the 250 nm wavelength QW is grown close to the n-side, it acts as an indicator for the presence of holes. In addition, the number of 233 nm QWs was varied between two and twenty. Temperature dependend electroluminescence-measurements have been performed on all samples. Analysis of the spectra shows a decrease in 250 nm intensity with increasing number of 233 nm QWs, due to capturing and confinement of the holes by 233 nm QWs. Comparing pulsed with continuous wave measurements for different current densities shows a significant decrease of intensity due to heating for the short wavelength QWs. Cooling of the LEDs down to 100 K reduces mobility of holes, which leads to a increase of the power ratio of 233 nm radiation to 250 nm radiation.

HL 52.3 Fri 10:00 EW 015

**Impact of overgrowth conditions on characteristics of tunnel-junction LEDs** — •Christoph Berger, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

The implementation of tunnel-junctions (TJs) on the p-side of blue light emitting diodes (LEDs) offers an exciting way to realize transparent, highly conductive electrodes for enhanced hole injection, better current spreading and higher efficiency. We realized TJ-LEDs by growth of a 100 nm thick GaN:Ge layer with an electron concentration of $1x10^{20}$ $cm^{-3}$ on top of the GaN:Mg layer in a continuous growth process by MOVPE. No in-situ or ex-situ activation steps were carried out and even 1 $mm^2$ LEDs show homogeneous light emission with improved output power. We propose that the activation of the p-GaN occurs during overgrowth with the GaN:Ge layer. Although n-doped GaN is known to block hydrogen diffusion, we assume an out-diffusion of $H_2$ promoted by V-pits that are formed during GaN:Ge growth in nitrogen ambient. Growing an additional GaN:Si layer in $H_2$-ambient on top of the TJ-LED for surface smoothening detoriates the optical and electrical characteristics of the device, suggesting repassivation of p-GaN by $H_2$ diffusion through the GaN:Ge layer. We will show results of different overgrowth schemes to elucidate the activation process for further improvement of device characteristics especially with regard to cascaded LEDs

HL 52.4 Fri 10:15 EW 015

**A pressure sensitive silicon field effect transistor comprising a buffer-free piezoelectric $Al_{0.72}Sc_{0.28}N$ layer** — •Rafael Ashkrizzadeh[1], Ole Gronenberg[2], Adrian Petraru[1], Lorenz Kienle[2,3], and Hermann Kohlstedt[1,3] — [1]Nanoelectronics, Faculty of Engineering, Kiel University, Germany — [2]Synthesis and Real Structure Group, Faculty of Engineering, Kiel University, Germany — [3]Kiel NanoSurface and Interface Science KiNSIS, Kiel University, Germany

In this work, we present a n-channel MISFET which consist of a 100 nm thick piezoelectric $Al_{0.72}Sc_{0.28}N$ layer in the gate stack. The functional $Al_{0.72}Sc_{0.28}N$ layer was deposited by dc/rf sputtering directly, i.e. buffer-free, on the Si-channel. The structure of the piezoelectric $Al_{0.72}Sc_{0.28}N$ layer as deposited on Si was investigated by wide-range reciprocal space mapping (RSM) and pole figures. Cross-sections taken of the gate stack were analyzed by Transmission Electron Microscopy (TEM) and chemical analyses by Energy Electron Loss Spectroscopy (EELS) line-scans, showed no indication of a residual interfacial layer.

HL 52.5 Fri 10:30 EW 015

**Heterostructure design of 233 nm far-UVC LEDs with varied DPD layer thickness** — •Paula Vierck[1], Jakob Höpfner[1], Marcel Schilling[1], Massimo Grigoletto[2], Tim Wernicke[1], and Michael Kneissl[1] — [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 have applications in skin safe disinfection and gas sensing. However, their internal quantum efficiency (IQE) is still low compared to LEDs emitting in the visible spectral range. Magnesium is commonly used as the p-type dopant in AlGaN materials. It has a high ionization energy which increases even more with rising aluminum content resulting in low hole concentrations and high series resistances particularly in devices with short emission wavelengths. Instead of doping the p-AlGaN layers with magnesium, a distributed-polarization doping (DPD) layer can be used to realize a Mg-free p-side. By composition grading from an AlN-layer to an 80% AlGaN, fixed negative space charges are introduced generating free holes in the DPD-AlGaN layer which enables a highly conductive and UV-transparent p-side. In this work, a series of 233 nm LEDs was simulated comparing two different drift diffusion simulation tools while varying the DPD thickness between 50 nm and 350 nm. The impact of the DPD thickness on the devices performance and its band structure were investigated, indicating a rising IQE with decreasing DPD thickness with a maximum value of 0.28 % at 54 $A/cm^3$ for a 50 nm thick DPD.

**15 min. break**

HL 52.6 Fri 11:00 EW 015

**Optically pumped UVC VCSELs** — •Estrella Torres Vasquez[1], Joachim Ciers[1], Nelson Rebelo[1], Filip Hjort[1], Michael Bergmann[1], Sarina Graupeter[2], Giulia Cardinali[2], Johannes Enslin[2], Tim Wernicke[2], Michael Kneissl[2,3], and Åsa Haglund[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Technical University of Berlin, Berlin, Germany — [3]Ferdinand-Braun-Institut (FBH), Berlin, Germany

We demonstrate optically pumped ultraviolet-C (UVC <280 nm) vertical-cavity surface-emitting lasers (VCSELs) with an accurate cavity length control including a smooth etched N-polar surface. This was enabled by photo-assisted electrochemical etching of an $Al_{0.45}Ga_{0.55}N$ sacrificial layer with a Si doping of $4\times10^{19}$ $cm^{-3}$. The VCSEL consists of an AlN cavity with 5 $Al_{0.30}Ga_{0.70}N/Al_{0.70}Ga_{0.3}N$ quantum wells and $SiO_2/HfO_2$ distributed Bragg reflectors. Photoluminescence measurements show a non-linear output power vs. pump power with a threshold pump power density down to 2 $MW/cm^2$ (incident power density) and a strong spectral narrowing down to 50 pm linewidth above threshold. The angular-resolved far-field spectrum changes from parabolic to non-dispersive around threshold with a 9° full width at half maximum. The main lasing wavelength only varies ∼1.2 nm between different UVC VCSELs across a 1.4 mm x 0.9 mm area, indicating an excellent cavity length control.

HL 52.7 Fri 11:15 EW 015

**Temperature dependent electroluminescence studies of the influence of the electron blocking layer thickness on the emission characteristics of deep ultraviolet light emitting diodes** — •Jakob Höpfner[1], Fabio Steyer[1], Marcel Schilling[1], Anton Muhin[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

Earlier studies have shown that a low current injection efficiency (CIE) is partly responsible for the poor external quantum efficiencies (EQE) of AlGaN-based deep ultraviolet light emitting diodes (DUV-LEDs). In particular, the hole injection and the carrier distribution in the AlGaN multi quantum well (MQW) active region is not well understood. In order to get a better insight we have performed temperature dependent electroluminescence (EL) investigations of three-fold AlGaN MQW LEDs with a variation of the electron blocking layer (EBL) thickness. We found an optimal EBL thickness of 12 nm for the highest external quantum efficiency of our DUV-LEDs. Additionaly we observed no voltage penalty by increasing the EBL-thickness. Temperature dependent measurements revealed a difference in high temperature stability with changed electron blocking layer thickness of our devices. These experimental results are also supported by by drift diffusion simulations and enable us to further understand the carrier transport in DUV-LED heterostructures.

HL 52.8 Fri 11:30 EW 015

**Facet degradation mechanisms of InGaN-based laser diodes emitting around 420 nm** — •Erik Freier, Jos Boschker, Johannes Glaab, Anna Mogilatenko, Carsten Netzel, Martin Guttmann, Ji Hye Kang, Saad Makhladi, and Sven Einfeldt — Ferdinand-Braun-Institut (FBH), Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

There are numerous possible applications for InGaN-based laser diodes in the field of metrology and sensing. One example is an external cavity diode laser for a rubidium-based optical atomic clock for use in space. In order to realize such an experiment, a diode laser with an emission wavelength of 420 nm with high reliability and stability in terms of emitted output power and beam direction is a basic prerequisite. The facet coating has a significant influence on the laser properties. In long-term cw operation, we tested the reliability of ridge waveguide lasers with various facet coating material systems consisting of Al2O3, SiO2, TiO2, and Ta2O5, respectively, in different atmospheres. The facet degradation was investigated using scanning and transmission electron microscopy combined with energy dispersive x-ray spectroscopy. As a general effect, we observe the formation of a SiOx layer of several 100 nm thickness on the output facet during laser emission. This leads to fluctuations in the output power of the diode laser. We discuss several options to suppress this effect including the use of different coating material combinations, atmospheres and aging conditions. We present strategies to fabricate long-term stable facets of blue-violet lasers with a stable laser emission of 20 mW for thousands of hours.

HL 52.9 Fri 11:45 EW 015

**Influence of the MQW heterostructure variations on the efficiency of AlGaN-based DUV LEDs** — •Markus A. Blonski[1], Anton Muhin[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[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

Deep ultraviolet (DUV) light emitting diodes (LEDs) with emission wavelengths shorter than 235 nm exhibit an external quantum efficiency (EQE) below 2 %. The EQE is comprised by the product of carrier injection efficiency (CIE), light extraction efficiency (LEE) and radiative recombination efficiency (RRE). In this work we investigate the RRE of epitaxially grown DUV-LEDs emitting below 235 nm using the Titkov-Dai method through a fit of the EQE. The impact of AlGaN quantum well thickness, AlGaN barrier thickness and Al molar fraction on the RRE of DUV-LEDs is investigated. To apply the Titkov-Dai method, reliable EQE measurements across a wide range of current densities from few $mA/cm^2$ to few hundred $A/cm^2$ are required. Accurate measurements at low currents are performed in continuous wave (cw) operation. To exclude Joule heating of the device at high currents we use pulsed electroluminescence spectroscopy with the parameters being determined by varying the pulse width, frequency and delay time between pulsed measurements and comparing them to cw measurements. At currents above 5 mA, pulsed measurements are required to suppress heating and aging of the LEDs, and for currents below 1 mA cw measurements were used to achieve lower noise levels.

# HL 53: 2D Materials and Heterostructures: (Twisted) Bilayers (joint session HL/TT)

Time: Friday 9:30–12:15 Location: EW 201

HL 53.1 Fri 9:30 EW 201

**Lattice relaxation, electronic structure and continuum model for twisted bilayer MoTe2** — •Ning Mao[1], Cheng Xu[2,3], Jiangxu Li[2], Ting Bao[3], Peitao Liu[4], Yong Xu[3], Claudia Felser[1], Liang Fu[5], and Yang Zhang[2,6] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA — [3]Department of Physics, Tsinghua University, Beijing 100084, China — [4]Institute of Metal Research, Chinese Academy of Sciences, 110016 Shenyang, China — [5]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [6]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Our study delves into the effect of lattice relaxation on the moiré band structures of twisted bilayer MoTe2, implemented by large-scale first-principles calculations and transfer learning neural network. Throughout our study, we have incorporated two van der Waals correction methods: the Grimme D2 method and a density-dependent energy correction. Notably, the latter method demonstrates a continuous evolution of bandwidth with respect to twist angles. Our findings reveal the critical role of in-plane lattice displacements, which generate substantial pseudomagnetic fields, reaching up to 250 T. Building on these insights, we have developed a comprehensive continuum model with a single set of parameters for a wide range of twist angles, providing a useful starting point for many-body simulation.

HL 53.2 Fri 9:45 EW 201

**Twist disorder in $tWSe_2$: Insights from Lateral Force Microscopy and Raman Spectroscopy** — •Nicolai-Leonid Bathen[1], Rami Dana[2], Hendrik Lambers[1], Nihit Saigal[1], Julian Klein[2], Frances M. Ross[2], and Ursula Wurstbauer[1] — [1]University of Münster, Münster, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, United States

Bilayers of twisted transition metal dichalcogenides (TMDCs) form moiré hybridized lattices resulting in moiré minibands [1] which leads to the capability to host correlated quantum phases [2] and to simulate Mott-Hubbard physics [3]. These properties vary strongly with the local twist angle configuration due to changes in the moiré cell size, symmetry and long-range disorder. Here we unravel the formation of moiré lattices and local disorder in the twist angle in twisted $WSe_2$ homo-bilayers ($tWSe_2$) by lateral force microscopy in ambient providing atomic resolution. We studied several $tWSe_2$ bilayers with a large variety in the nominal twist angle of 3° to 11° and find a surprisingly large variation in twist angle up to 1° within less than a micrometer distance. We contrast those findings with low-frequency Raman measurements sensitive to interlayer coupling and we will discuss consequences of the local twist disorder for collective inter-moiré band excitations studied by resonant inelastic light scattering [1].

[1] N. Saigal et al., arXiv 2310 14417 (2023) [2] N. P. Wilson et al., Nature 599, 383-392 (2021) [3] S. Ryee and T. O. Wehling, Nano Lett. 23 (2), 573-579 (2023) [4] Y. Song and E. Meyer, ACS Langmuir 39, 15409 (2023)

HL 53.3 Fri 10:00 EW 201

**Electrical tuning of moiré excitons in $MoSe_2$ bilayers** — •Joakim Hagel[1], Samuel Brem[2], and Ermin Malic[2,1] — [1]Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden — [2]Department of Physics, Philipps University of Marburg, 35037 Marburg, Germany

Recent advances in the field of vertically stacked 2D materials have revealed a rich exciton landscape. In particular, it has been demonstrated that out-of-plane electrical fields can be used to tune the spectral position of spatially separated interlayer excitons. Other studies have shown that there is a strong hybridization of exciton states, resulting from the mixing of electronic states in both layers. However, the connection between the twist-angle dependent hybridization and field-induced energy shifts has remained in the dark. Here, we investigate on a microscopic footing the interplay of electrical and twist-angle tuning of moiré excitons in homobilayers [1,2]. We reveal distinct energy regions in PL spectra that are clearly dominated by either intralayer or interlayer excitons, or even dark excitons [1]. Consequently, we predict twist-angle-dependent critical electrical fields at which the material is being transformed from a direct into an indirect semiconductor [1]. Our work provides new microscopic insights into experimentally accessible knobs to significantly tune the moiré exciton physics in atomically thin nanomaterials.

[1] J. Hagel, S. Brem, E. Malic, 2023 2D Mater. 10 014013

[2] Tagarelli, F., Lopriore, E., Erkensten, D. et al. Nat. Photon. 17, 615-621 (2023)

HL 53.4 Fri 10:15 EW 201

**Exciton-polaritons in twisted-bilayer heterostructures** — •Francesco Troisi[1], Hannes Huebener[1], Angel Rubio[1,3], and Simone Latini[2] — [1]MPSD, Hamburg, Germany — [2]Department of Physics, DTU, Lyngby, Denmark — [3]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, NYC, USA

2D materials, such as TMDs, have attracted significant attention due to their unique electronic properties, such as tunable bandgap, high emission efficiency, and a strong excitonic binding allowing the formation of stable excitons at room temperature. Excitons in multilayer TMD structures are the object of great interest, as we find both inter- and intra-layer excitons, which give rise to a response at different energies. Previous works show that it is possible to tune the Moiré potential to control their localization, which influences the optical properties.

In the quest to understand and control excitons in novel environments, this study focuses on excitonic behavior for a twisted bilayer MoSe2/WSe2 heterostructure in an optical cavity. Our goal is to produce an all-optical Moiré-like exciton confinement by tuning the cavity. Optical cavities provide a promising approach to controlling material properties by coupling the electronic transitions in the material to the confined photons inside the cavity, which implies photonic and excitonic states cannot be separated. The so-called exciton-polariton states are obtained. In the strong coupling regime, one needs to go beyond the perturbative approach to treat the light-matter problem.

This study utilizes the full diagonalization of the QED problem built from the Wannier equation in k-space and the Moiré potential.

HL 53.5 Fri 10:30 EW 201

**Investigating the orbital dependence of the superlattice potential in Moiré semiconductors with NanoARPES** — •Gianmarco Gatti[1], Julia Issing[1], Dario Rossi[2], Louk Rademaker[2], Anna Tamai[1], and Felix Baumberger[1] — [1]Department of Quantum Matter Physics, University of Geneva, Geneva, 1211, Switzerland — [2]Department of Theoretical Physics, University of Geneva, Geneva, 1211, Switzerland

Moiré semiconductors emerged as tunable quantum simulators for strongly correlated phases. The single-particle low-energy physics is ruled by the moiré-periodic superpotential that develops by twisting or stacking layers with different lattice parameters. Signatures of this modulation are observed in the spectral function measured by angle-resolved photoemission spectroscopy (ARPES) in the form of replicas and gaps opening at the nascent zone boundary. In twisted bilayer transition metal dichalcogenides (TMDs), flat bands are reported at the Brillouin zone center and their dispersion is associated to the effective moiré potential experienced by electronic states with large out-of-plane orbital character. Here, we extend this analysis and present the orbital and wave vector dependence of this interaction over the whole Brillouin zone by comparing quantitatively our ARPES data on a TMD heterobilayer with an extended tight-binding model. Our results set the fundaments for future spectroscopic studies of the electronic correlations in moiré systems.

HL 53.6 Fri 10:45 EW 201

**Confocal SHG microscopy of twisted bilayers of $MoS_2$** — •Nikita V. Siverin[1], Daniel J. Gillard[2], Dmitri R. Yakovlev[1], Alexander I. Tartakovskii[2], and Manfred Bayer[1] — [1]TU Dortmund, Dortmund, Germany — [2]The University of Sheffield, Sheffield, UK

We investigate the crystal and exciton symmetries in twisted $MoS_2$ bilayer flakes using second harmonic generation (SHG). By measuring and modeling the full dependence of the SHG signal on the linear polarization angles of incident and emitted light we reveal the underlying mechanisms of SHG. Our method employs a confocal microscopy

setup, allowing for spectroscopic investigations of different excitonic resonances.

Twisting layers of 2D materials is a familiar technique that produces a superlattice and gives rise to the phenomena called moiré structure inducing changes in optical properties.

We measured different regions of overlapping flakes: monolayer, twisted monolayers, bilayer and twisted bilayers. We observe strong SHG signal from monolayers and we can measure twisted angle by polarization anisotropies of the SHG signal. According to group theory, SHG is forbidden in bilayers, but we observe small signal with rotational anisotropy deviating from the one for monolayers.

**15 min. break**

**Invited Talk** HL 53.7 Fri 11:15 EW 201

**Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene** — •Anna Seiler[1], Nils Jacobsen[1], Martin Statz[1], Fabian Geisenhof[2], Felix Winterer[2], Isabell Weimer[1], Tianyi Xu[3], Zhiyu Dong[4], Leonid Levitov[4], Fan Zhang[3], and Thomas Weitz[1] — [1]University of Göttingen — [2]Ludwig-Maximilians-Universität München — [3]University of Texas at Dallas — [4]Massachusetts Institute of Technology

The bandstructure of naturally occurring Bernal bilayer graphene exhibits four linearly-dispersed Dirac cones but changes drastically when large electric displacement fields are applied across the two layers. Here, tunable van Hove singularities lead to the emergence of complex correlated states. We observe experimental signatures consistent with various interaction-driven phases, including the fractional metals of Stoner type [1, 2]. More prominently, we find competing nontrivial insulating and metallic phases at hole doping that exhibit intriguing temperature dependences and nonlinear I-V characteristics at zero magnetic fields [1]. In addition, we report a novel interaction-driven behaviour in the Stoner phases in the electron-doped regime electric-field gapped Bernal bilayer graphene [2]. Specifically, we reveal that the spin- and valley-polarized phases exhibit an insulator-like temperature dependence of the conductance that challenges the conventional picture of metallic Stoner magnetism.

[1] A. M. Seiler et al., Nature 608, 298-302 (2022)
[2] A. M. Seiler et al., arXiv:2308.00827 (2023)

HL 53.8 Fri 11:45 EW 201

**Valley transport assisted by Fermi surface warping** — Josep Ingla-Aynés[1], •Antonio L. R. Manesco[1], Talieh S. Ghiasi[1], Serhii Volosheniuk[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Herre S. J. van der Zant[1] — [1]Kavli Institute of Nanoscience, Delft University of Technology, Netherlands — [2]Research Center for Electronic and Optical Materials, National Institute for Materials Science, Japan — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan

Valleys are distinct energy extrema in a band structure. Graphene has a band structure with two valleys at distinct high-symmetry points. The large momentum separation of these points suppresses intervalley scattering in ballistic devices. However, even in ballistic devices, valley coherence is limited by atomically-sharp edge disorder. Gate-defined bilayer graphene devices overcome this limitation and enable the observation of valley coherent phenomena. In this work, we explored ballistic electron transport in multiterminal bilayer graphene devices. We observed specular electron-focusing between gate-defined quantum point contacts, suggesting that smooth edges preserve valley polarization. Moreover, trigonal warping of the Fermi surface causes valley-dependent electron jetting, which we detected with magnetic collimation. Our results show two current peaks in the collector signal at opposite magnetic fields, consistent with the injection of two valley-polarized electron jets. Since the valley polarization of the electron current depends on the magnetic field, collimation devices are current sources with tuneable valley polarization.

HL 53.9 Fri 12:00 EW 201

**Gate screening of Coulomb interactions in Bernal bilayer graphene** — •Isabell Weimer[1], Anna Seiler[1], Dong Zhao[2], Jurgen Smet[2], and R. Thomas Weitz[1] — [1]1st Institute of Physics, Faculty of Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]MPI for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Measurements on dual gated, hexagonal Boron Nitride (hBN) encapsulated Bernal bilayer graphene samples, have revealed a complex phase space for Bernal bilayer graphene, including numerous Stoner metals, a correlated insulator consistent with a Wigner-Hall crystal [1] and superconducting behavior [2].

We have investigated the influence of the gate induced Coulomb interaction screening [3] on the appearance of previously reported correlated phases in gated Bernal bilayer graphene devices, using the thickness of the dielectric hBN spacing layers as variable parameter. In direct comparison of devices studied here, which are characterized by a comparably thin h-BN layer, with the data of Seiler et. al. , we observed behavior, which is supportive of an effectively lowered magnitude of Coulomb interactions. Additionally, three features in the transport data were identified, which could potentially be indicative of phases, not reported in [1] and [2].

References: [1] Seiler, Anna M., et al. Nature 608.7922 (2022): 298-302. [2] Zhou, Haoxin, et al. Science 375.6582 (2022): 774-778. [3] Kim, Minsoo, et al. Nature communications 11.1 (2020): 2339.

## HL 54: Focus Session: Evolution of Topological Materials into Superconducting Nanodevices III (joint session HL/TT)

The focus session intends to span the arc between topological materials and superconducting nanodevices, both experimentally and theoretically. Such structures are interesting for applications in future topological quantum circuits. In recent years, the number of topological materials and the knowledge about them has rapidly increased. As part of the focus session, material properties of layered systems made of topological materials, especially in combination with superconductors, are discussed. On the other hand, the special challenges in the nanofabrication of these materials for use in future topological quantum processors are addressed. Another focus is the quantum transport in nanoscale hybrid structures.

Organized by Thomas Schäpers, Philipp Rüßmann, and Peter Schüffelgen

Time: Friday 9:30–12:45 Location: EW 202

**Invited Talk** HL 54.1 Fri 9:30 EW 202

**Tunneling spectroscopy of a phase-tunable topological insulator Josephson junction** — •Jakob Schluck[1], Ella N. Nikodem[1], Anton Montag[2], Alexander Ziesen[2], Mahasweta Bagchi[1], Zhiwei Wang[1], Fabian Hassler[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne — [2]JARA-Institute for Quantum Information, RWTH Aachen University

Topological superconductivity is predicted to be realized in a topological insulator proximitized by an s-wave superconductor [1]. In such a system, vortices host Majorana zero modes - quasiparticle excitations obeying non-Abelian exchange statistics that could have important applications as topological qubits.

Here we present our experimental findings concerning the bound state spectrum of topological insulator Josephson junctions. We locally probe the density of states through tunnel contacts made on top of the junction, while tuning the phase difference across it by applying an external magnetic field.

We find a periodic filling of the induced gap, with states reaching zero energy for a local phase difference of $\pi$. Taking the phase gradient along the junction into account, we interpret those as signatures of

Majorana zero modes bound to the $\pi$-phase boundary [2]. We will discuss their stability with respect to the chemical potential and possible trivial origins.

[1] Liang Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008) [2] A. C. Potter and L. Fu, Phys. Rev. B 88, 121109 (2013).

**Invited Talk** HL 54.2 Fri 10:00 EW 202

**Robust Majorana modes in topological material-based nanoelectronic hybrid devices** — •Kristof Moors — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

Majorana modes have the potential to be used as robust carriers of quantum information for future fault-tolerant quantum information processing applications. While their realization in various condensed matter systems is well understood in principle, realistic conditions (with, e.g., disorder or imperfections) can complicate their formation as well as experimental verification in practice. I will present recent modeling and simulation results on two promising platforms for Majorana devices: magnetic and nonmagnetic topological insulator nanoribbons with proximity-induced superconductivity, respectively. These platforms have distinct advantages for a robust realization of Majorana modes by forming them out of their proximitized and topologically protected surface or edge states. In this way, a higher tolerance with respect to disorder and less finetuned conditions can be obtained as compared to alternative platforms. I will discuss the topological phase with well-separated Majorana modes in such systems under realistic conditions, the robustness against disorder, and distinct signatures in spectroscopy and transport experiments. I will also comment on the latest status regarding the experimental development.

**Invited Talk** HL 54.3 Fri 10:30 EW 202

**Thermal and electric response of superconducting topological materials; are Majorana states more widespread than expected?** — •Ewelina Hankiewicz — Institute for Theoretical Physics, Uni Würzburg, Germany

In this talk, we will discuss different Josephson junctions based on semimetals, metals and topological insulators proximitized with s-wave superconductors. We show that thermal response can be more sensitive to Majorana bound states than an electrical response [1,2]. Moreover, due to the 4pi periodicity of topological Josephson junctions, the thermal engines built on them are more efficient as the ones on the classical Josephson junctions [3].

Furthermore, we predict that the s-wave superconductivity proximitized j=3/2 particles in 2D Luttinger materials are able to host Majorana bound states even in the absence of Dresselhaus and Rashba spin-orbit couplings [4]. This originates from the hybridization of the light and heavy hole bands of the j=3/2 states in combination with the superconducting pairing. We predict that Majorana bound states should be seen in many classes of materials like p-doped GaAs and bulk HgTe [4].

[1] A. G. Bauer et al. Phys. Rev. B 104, L201410 (2021). [2] R. L. Klees, D. Gresta, J. Sturm, L. W. Molenkamp, and E. M. Hankiewicz arXiv:2306.17845 (2023). [3] B. Scharf, A. Braggio, E. Strambini, F. Giazotto, E. M. Hankiewicz, Communications Physics 3, 198 (2020). [4] J.-B. Mayer, M. A. Sierra, and E. M. Hankiewicz, Phys. Rev. B 105, 224513 (2022).

**15 min. break**

**Invited Talk** HL 54.4 Fri 11:15 EW 202

**Tunable Josephson coupling in HgTe nanodevices** — •Martin P. Stehno — Physikalisches Institut EP3 und Institut für Topologische Isolatoren, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Mercury telluride offers access to a variety of topological phases in a single material system. This opens up opportunities for disentangling the complex interplay of band structure effects, interface preparation, and phase dynamics that characterize the Josephson effect in topological insulator nanodevices. We study a new generation of gate-tunable Josephson junctions with weak links fabricated from 2D and 3D topological insulator HgTe. These devices feature ballistic transport over a wide range of carrier densities and allow us to map out the Josephson coupling of topological states and bulk modes using a combination of quantum transport methods, supercurrent interference, and microwave spectroscopy. By adding a gated constriction into a 2D topological insulator weak link, we create a quantum point contact (QPC) that allows us to study the ac Josephson effect as a function of the number of open channels. As we deplete the constriction further, we explore proximity-induced superconductivity in the quantum spin Hall edge channels and in the regime of the recently discovered 0.5-anomaly in HgTe QPC devices.

**Invited Talk** HL 54.5 Fri 11:45 EW 202

**Superconducting proximity effect in topological Dirac materials** — •Chuan Li[1], Anqi Wang[2], Caizhen Li[2], Chhunguang Chu[2], Zhimin Liao[2], and Alexander Brinkman[1] — [1]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands. — [2]State Key Laboratory for Mesoscopic Physics and Frontiers Science Center for Nano-optoelectronics, Peking University, 100871 Beijing, China

Inducing superconductivity in topological materials stimulates the formation of novel quantum states of matter. Besides the original prediction in 3D topological insulators, the notion of topological phases has been generalized to different dimensions and extended to the higher-order states.

In the last few years, our research has demonstrated the possibility of realizing the topological superconductivity in engineered 3D topological insulators, 3D Dirac semimetals [1,2], and their 1D hinge states. Particularly, Cd3As2 is predicted to be a higher-order topological semimetal, possessing three-dimensional bulk Dirac fermions, two-dimensional Fermi arcs [3], and one-dimensional hinge states [4] or non-Hermitian states [5]. These topological states have different characteristic length scales in electronic transport. We show that the superconducting proximity effect can be a sensitive probe for distinguishing these states.

[1] Li, C. et al. Nat. Mater. 17, 875 (2018). [2] Wang, A. Q. et al. PRL (2018). [3] Li, C.-Z. et al. Nat. Commun.(2020). [4] Li, C.-Z. et al. PRL (2020). [5] C. G. Chu, et al., Nat. Commun. (2023).

**Invited Talk** HL 54.6 Fri 12:15 EW 202

**Exploring Josephson Junctions made of Topological Insulator Wires and Superconductors** — •Dieter Weiss — Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg

Topological insulator (TI) nanowires in proximity to conventional superconductors provide a tunable platform to realize topological superconductivity and Majorana bound states (MBS) [1]. Tuning is achieved by an axial magnetic flux $\phi$ which transforms the system from trivial at $\phi$ =0 to topologically non-trivial when a magnetic flux quantum $\phi_0 = h/2e$ threads the wire cross section. Here we study the supercurrent $I_C$ and its periodicity on the superconducting phase as a function of the axial magnetic field using Josephson junctions made of strained HgTe wires (the TI) with Nb contacts. Depending on the transparency of the contacts we observe either a monotonically decreasing $I_C$ with increasing $B$ for high transparency or $h/2e$, $h/4e$, and even $h/8$e periodic oscillations of the supercurrent for samples with lower transparency [2]. Samples with high transparency exhibit $4\pi$ periodic supercurrents, a signature of MBS [3]. I will discuss the significance of these signatures and the origin of the flux-periodic oscillations.

Work done in collaboration with Ralf Fischer, Wolfgang Himmler, Jordi Picó-Cortés, Jacob Fuchs, Michael Barth, Cosimo Gorini, Klaus Richter, Gloria Platero, Milena Grifoni, Dmitriy A. Kozlov, Nikolay N. Mikhailov, Sergey A. Dvoretsky, and Christoph Strunk.

[1] A. Cook and M. Franz, Phys. Rev. B 84, 201105(R) (2011)
[2] W. Himmler et al., Phys. Rev. Res. 5, 043021 (2023)
[3] R. Fischer et al., Phys. Rev. Res. 4, 013087 (2022)

# HL 55: Perovskite and Photovoltaics III (joint session HL/KFM)

Time: Friday 9:30–13:00 Location: EW 203

HL 55.1 Fri 9:30 EW 203

**Data-efficient machine learning for perovksite alloys** — •Jarno Laakso, Henrietta Homm, and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Perovskite solar cells are highly efficient, but their commercialization has been hindered by toxicity and lack of stability. Compositional engineering can mitigate these problems [1], but the complexity of the perovskite materials space makes the search for an optimal solar cell material challenging. We previously demonstrated how machine learning (ML) can accelerate property predictions for the perovskite alloy $CsPb(Cl/Br)_3$ [2]. However, the extensive density functional theory (DFT) calculations required for model training prevent applications to more complex materials. Here, we facilitate model training with a data-efficient scheme, validated on $CsPb(Cl/Br)_3$ data and extended to the ternary alloy $CsSn(Cl/Br/I)_3$.

Our approach employs clustering to build a compact but diverse initial data set of atomic structures. We then apply a two-stage active learning approach to first improve the robustness of the ML-based structure relaxations and then fine-tune the accuracy near equilibrium structures. Tests for $CsPb(Cl/Br)_3$ reveal that our scheme reduces the number of required DFT calculations during model training by up to 50%. The fitted model for $CsSn(Cl/Br/I)_3$ is robust, with all ML-based structure relaxations converging in our tests. The relaxations are also highly accurate, having an average error of 0.5 meV/atom.

[1] *iScience* **23**, 101359 (2020). [2] *Phys. Rev. Mater.* **6**, 113801 (2022).

HL 55.2 Fri 9:45 EW 203

**Passivation and Charge Carrier Selectivity Optimization for Narrow Bandgap Perovskite Solar Cells** — •Athanasia Vicha, Georgios Loukeris, Markus Kohlstädt, Uli Würfel, and Andreas Bett — Fraunhofer ISE, Freiburg im Breisgau, Germany

This study aims to enhance narrow bandgap perovskite solar cells for all-perovskite tandem applications. Initial efforts focused on bulk passivation of the perovskite layer. The combination of two additives, Methylammonium chloride and Lead thiocyanate, increased Voc up to 0.82V and Jsc to 31mA/cm^2. Glycine hydrochloride improved result reproducibility leading to a favourable FF, and increasing Thiourea concentration simultaneously raised Jsc. Further optimizations and the effects of additive combinations will be presented. Concurrently, this study investigates the selectivity of the hole transport layer/perovskite interface. Thus, we examined substituting an aqueous PEDOT:PSS formulation for a solvent-based one to address water-induced degradations in the underlying perovskite layer in all-perovskite tandem devices. Preliminary assessments on single-junction narrow bandgap solar cells using solvent-based PEDOT yielded a notable 16% Voc increase compared to aqueous PEDOT:PSS. However, this rise in Voc results in a significant 23% Jsc reduction. In response, we explored strategies to boost Jsc by varying the PEDOT thickness. In thinner layers, Jsc exceeds the one of PEDOT:PSS-based cells, aligning with simulations. This research outcome provides valuable insights into optimizing passivation and enhancing selectivity in narrow bandgap perovskite solar cells.

HL 55.3 Fri 10:00 EW 203

**Understanding and mitigating atomic oxygen-induced degradation of Perovskite solar cells for near-earth space applications** — •Biruk Seid — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

Atomic oxygen (AtOx) in low-Earth orbit is known to etch, corrode, and form metal oxide on the metal contact with PSC devices. To mitigate this issue, we report the applicability of thermally evaporated 0.7*m silicon oxide (SiOx) encapsulation as an AtOx barrier for triple-cation PSC. Moreover, the AtOx-induced degradation mechanism of phenethylammonium iodide (PEAI)-passivated and non-passivated devices are discussed and analyzed. We found that after a total exposure duration of 120 minutes, the SiOx-encapsulated cells maintained over 97% of their initial power conversion efficiency (PCE), regardless of the device type (passivated or non-passivated). In contrast, in the case of unencapsulated devices, PCEs for non-passivated and PEAI-passivated devices the PCE declined to a maximum value of 43% and 62%, respectively. In non-passivated and unencapsulated devices, AtOx has no impact on the short-circuit current density (JSC) but degrades the fill factor (FF) and open circuit voltage (VOC). In PEAI-passivated devices, the JSC additionally degrades by almost 35%. perovskite was not the origin of PCE degradation. Instead, inefficient charge extraction and mobile ions, due to a swiftly degrading PEAI interlayer are the primary causes of AtOx-induced device performance degradation in passivated devices, whereas a large ionic FF loss limits non-passivated devices.

HL 55.4 Fri 10:15 EW 203

**Understanding and mitigating atomic oxygen-induced degradation of Perovskite solar cells for near-earth space applications** — •Biruk Seid — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

Atomic oxygen (AtOx) in low-Earth orbit is known to etch, corrode, and form metal oxide on the metal contact with PSC devices. To mitigate this issue, we report the applicability of thermally evaporated 0.7*m silicon oxide (SiOx) encapsulation as an AtOx barrier for triple-cation PSC. Moreover, the AtOx-induced degradation mechanism of phenethylammonium iodide (PEAI)-passivated and non-passivated devices are discussed and analyzed. We found that after a total exposure duration of 120 minutes, the SiOx-encapsulated cells maintained over 97% of their initial power conversion efficiency (PCE), regardless of the device type (passivated or non-passivated). In contrast, in the case of unencapsulated devices, PCEs for non-passivated and PEAI-passivated devices the PCE declined to a maximum value of 43% and 62%, respectively. In non-passivated and unencapsulated devices, AtOx has no impact on the short-circuit current density (JSC) but degrades the fill factor (FF) and open circuit voltage (VOC). In PEAI-passivated devices, the JSC additionally degrades by almost 35%. perovskite was not the origin of PCE degradation. Instead, inefficient charge extraction and mobile ions, due to a swiftly degrading PEAI interlayer are the primary causes of AtOx-induced device performance degradation in passivated devices, whereas a large ionic FF loss limits non-passivated devices with no change in transit time.

HL 55.5 Fri 10:30 EW 203

**Passivating Inorganic Interlayers at the Perovskite/$C_{60}$ Interface in Monolithic Perovskite Silicon Tandem Solar Cells** — •Johanna Modes[1,2], Patricia S.C. Schulze[1], Carl Eric Hartwig[4], Stefan Lange[4], Armin Richter[1], Juliane Borchert[1,3], and Andreas Bett[1,2] — [1]Fraunhofer ISE — [2]Albert-Ludwigs-Universität — [3]INATECH — [4]Fraunhofer CSP

Metal halide perovskites emerged in recent years as promising absorber materials for solar cells that can combine high power conversion efficiency with low production costs. Significant non-radiative charge carrier recombination occurs at the perovskite interface with the electron contact $C_{60}$, which prevents the full exploitation of the solar cell's potential. $C_{60}$ induces states within the band gap, lowers the quasi-Fermi level splitting, and limits the open circuit voltage ($V_{OC}$). Ultra-thin passivation layers at the perovskite/$C_{60}$ interface are used to reduce those losses. To enable industrial upscaling, our focus lies on inorganic passivation layers deposited via atomic layer deposition. An $AlO_x$ interlayer was developed that increases the i$V_{OC}$ up to 50 mV and improves the $V_{OC}$ for single-junction and tandem devices. To better understand the effects involved in this passivation, photoluminescence quantum yield (PLQY), angle-resolved X-ray photoelectron spectroscopy (ARXPS) and surface photovoltage (SPV) measurements were carried out. State-of-the-art perovskite solar cells using a $LiF_x$ passivation layer suffer from device degradation over time. Initial stability testing indicates that a thin $AlO_x$ passivation layer can improve device stability and can serve as an alternative to $LiF_x$.

HL 55.6 Fri 10:45 EW 203

**Analyzing defect thermodynamics of (Ag,Cu)$GaSe_2$ solar cell absorbers using a machine-learning interatomic potential** — •Vasilios Karanikolas, Delwin Perera, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

One of the most widely used absorber materials for thin-film solar cells is $Cu(In,Ga)Se_2$ (CIGS). Currently, CIGS yields the highest efficiencies within this technology and the addition of Ag has been found to

further improve the efficiency. The performance of the CIGS absorber, however, is also governed by defects, especially by the type and density of grain boundaries (GBs) [1].

In this work, we investigate the thermodynamic properties of GBs for $(Ag_{1-x}Cu_x)GaSe_2$ structures based on a machine learning interatomic potential (MLIP)[2]. The training dataset for the regression machine learning model is created by density functional theory (DFT) calculations. The MLIP allows us to perform molecular dynamics simulations for structurally complex GBs that are inaccessible by conventional electronic structure methods. In particular, we investigate the thermodynamic properties of symmetric GBs beyond Σ3 and include an analysis of silver segregation at the interfaces.

[1] D. Abou-Ras *et al.*, Acta Materialia **118**, 244-252 (2016).
[2] Y. Lysogorskiy *et al.*, npj Computational Materials **7**, 1 (2021).

**15 min. break**

HL 55.7 Fri 11:15 EW 203

**Halide segregation and ionic motion in lead-halide perovskites** — •Francisco Peña-Camargo, Felix Lang, and Martin Stolterfoht — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany

Halide segregation is a photoinduced phenomenon observed in perovskites with multiple halides at the X site of the ABX3 lattice. The evidence shows that the photoluminescence spectrum of the mixed phase red-shifts and increases its intensity in a timescale of minutes. On the other hand, it has been proven that mobile ions are present in cells in densities around 1016 cm-3, which is sufficient to screen the internal electric field, generating, among other effects, the hysteresis in the forward and reverse JV scans. The scan-speed dependence of hysteresis suggests that mobile ions have an effect on the cell performance mostly at a determined condition when the voltage sweep matches the ionic timescales. Here, by measuring the JV characteristic at different speeds with a novel technique called fast hysteresis (FH) from 10-2 to 104 V s-1, we quantify the ionic diffusion coefficient and conclude that the ionic motion happens in the seconds to minutes timescales. Moreover, using bias-assisted charge extraction (BACE) we are able to quantify the ionic volumetric density and confirm the ionic transient timescales. Based on that experimental evidence, it is plausible to link the ionic motion to halide segregation, particularly when it comes to the timescales which appear to match very well. This is also supported by the correlation of the ionic losses with the increasing Br/I ratio in triple-cation lead-based perovskite solar cells.

HL 55.8 Fri 11:30 EW 203

**Halide segregation and ionic motion in lead-halide perovskites** — •Francisco Peña-Camargo, Felix Lang, and Martin Stolterfoht — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany

Halide segregation is a photoinduced phenomenon observed in perovskites with multiple halides at the X site of the $ABX_3$ lattice. The evidence shows that the photoluminescence spectrum of the mixed phase red-shifts and increases its intensity in a timescale of minutes. On the other hand, it has been proven that mobile ions are present in cells in densities around $10^{16}$ $cm^{-3}$, which is sufficient to screen the internal electric field, generating, among other effects, the hysteresis in the forward and reverse JV scans. The scan-speed dependence of hysteresis suggests that mobile ions have an effect on the cell performance mostly at a determined condition when the voltage sweep matches the ionic timescales. Here, by measuring the JV characteristic at different speeds with a novel technique called fast hysteresis (FH) from $10^{-2}$ to $10^4$ V $s^{-1}$, we quantify the ionic diffusion coefficient and conclude that the ionic motion happens in the seconds to minutes timescales. Moreover, using bias-assisted charge extraction (BACE) we are able to quantify the ionic volumetric density and confirm the ionic transient timescales. Based on that experimental evidence, it is plausible to link the ionic motion to halide segregation, particularly when it comes to the timescales which appear to match very well. This is also supported by the correlation of the ionic losses with the increasing Br/I ratio in triple-cation lead-based perovskite solar cells.

HL 55.9 Fri 11:45 EW 203

**Assessing machine-learning force fields for defect calculations in halide perovskites** — •Frederico Delgado[1], Frederico Simões[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 excellent optoelectronic properties exhibited by bulk halide perovskites (HaPs) are important for their photovoltaic performance and have been extensively investigated. Despite this, the ubiquity of both point defects and extended ones like surfaces requires further careful examination of their impact on such properties. Precise investigations of dynamic effects in this context via ab-initio molecular dynamics imply large computational costs, especially when the need for accurate exchange correlation functionals arises. Therefore, in order to sample sufficiently long time scales and sufficiently large supercells, usage of on-the-fly machine learning (ML) forces fields appears to be particularly appealing. In this study, we investigate such defects and their dynamical properties in $CsPbBr_3$ using ML force fields. Our results can aid rationalizing the correlations between local structural dynamics and the observed optoelectronic behavior.

HL 55.10 Fri 12:00 EW 203

**Nanospectroscopy and ultrafast out-of-plane carrier dynamics in metal halide perovskites** — •Martin Zizlsperger[1], Svenja Nerreter[1], Qimu Yuan[2], Kilian B. Lohmann[2], Fabian Sandner[1], Felix Schiegl[1], Christian Meineke[1], Yaroslav Gerasimenko[1], Laura M. Herz[2], Thomas Siday[1,2], Markus A. Huber[1], Michael B. Johnston[2], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

The high efficiencies of metal halide perovskite solar cells have been associated with effective charge-carrier diffusion. Still, the characteristic nanograins and crystallographic disorder entailed in perovskite films hindered unraveling details of the vertical transport, calling for simultaneous experimental access to chemical composition, structural phase and ultrafast out-of-plane dynamics. Here, we promote depth-sensitive terahertz near-field nanospectroscopy to extreme subcycle time scales. In $FA_{0.83}Cs_{0.17}Pb(I_{1-x}Cl_x)_3$ films, we discern domains of the $\alpha$-phase from $\delta$-phase and $PbI_2$ nano-islands. Based on deep-subcycle time shifts of the scattered terahertz waveform after photoexcitation, we access the single-grain vertical diffusion. Despite topographic irregularities, diffusion is surprisingly homogeneous on sub-micrometer length scales, only varying between mesoscopic regions. Our approach linking nano-morphology with carrier dynamics may benefit all future optoelectronic devices using nanocrystalline materials.

HL 55.11 Fri 12:15 EW 203

**Comparison of the application of the TRMC technique for the characterization of crystalline silicon and perovskite solar cell absorber material and efficient surface passivation** — Arpana Singh[1], Biruk Alebachew Seid[2], Felix Lang[2], Marinus Kunst[3], and •Heinz-Christoph Neitzert[1] — [1]DIIN, Salerno University, 84084 Fisciano, Italy — [2]ROSI Freigeist Group, Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam-Golm, Germany — [3]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Time Resolved Microwave Conductivity (TRMC) as a contactless technique for the characterization of the charge carrier kinetics in photoconductive materials has been recently successfully applied for the characterization of perovskite thin films [1]. Charge carrier lifetimes depend strongly on excitation conditions, such as light intensity and wavelength. It is shown, how TRMC-measurements performed with excitation at low laser intensities and different wavelengths can give valuable information on the quality of the surface passivation of triple-cation, triple-anion Perovskite films by PEAI layers. A good correlation of the observed lifetime increase in the absorber films and the performance of the completed solar cells has been found. The results are compared to the characterization under identical measurement conditions of crystalline silicon wafers. Also in this case the influence of different passivation schemes on the charge carrier lifetime and on solar cell properties have been compared. [1] A. Marchioro, J. Teuscher, D. Friedrich, M. Kunst, R. van de Krol, T. Moehl, M. Grätzel and J. E. Moser, Nature Photonics 8, 250-256 (2014).

HL 55.12 Fri 12:30 EW 203

**The detrimental role of PbI2 at the interface between absorber and electron-transport layer in halide-perovskite solar cells** — •Dan Ralf Wargulski, Ke Xu, Steve Albrecht, and Daniel Abou-Ras — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

There is an ongoing discussion in the halide-perovskite community about the beneficial or harmful effects of PbI2 in halide-perovskite solar cells (HPSCs). One school praises PbI2 for its passivating and stabilizing properties, while the other aims at getting rid of excess PbI2, because it leads to decreased cell efficiencies and degraded long-term stability. How can such a contradiction exist? The effect of PbI2 depends on its location in the solar-cell stack and on the specific HPSC architecture used. When applied as top cells in tandem devices, HPSCs do not exhibit a n-i-p structure but an p-i-n structure, often called *inverted* HPSC structure. As a result, the top surface where PbI2 forms is not situated at the interface between the absorber and the hole-transport layer anymore, but at the interface to the electron-transport layer. This modifies considerably the effects of PbI2 on the device performance. The present work discusses the formation of PbI2 in HPSCs with slot-die-coated, triple-halide perovskite absorbers, which was investigated by means of correlative electron microscopy. Studying the changing PbI2 coverage of the halide-perovskite absorbers with varying annealing temperature, a model will be presented that explains the effects of the PbI2 precipitates on the open-circuit voltages and the fill factors of the HPSCs with inverted cell architecture.

HL 55.13 Fri 12:45 EW 203

**Stability Enhancement of Mixed-Cation Hybrid Halide Perovskites combining DFT-1/2 with SOC** — •Mohammad Moaddeli[1], Mansour Kanani[1,2], and Anna Grunebohm[3] — [1]Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — [2]Solar Energy Technology Development Center, Shiraz University, Shiraz, Iran — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Tunable band gaps, easy processing, composition engineering, and enhanced performance make mixed-cation perovskites promising as light absorbers in third generation solar cells. However, stability challenges remain in understanding the underlying mechanisms. This study emphasizes the importance of accurately predicting structural and electronic properties. While density functional theory (DFT) is the preferred method for addressing these, standard exchange-correlation functionals often fail to reproduce the band structure. Therefore, we propose the DFT-1/2 method, which is applied to single- and mixed-cation systems. We explore how the choice of the A-cation modifies the Pb-I scaffold. We find that the addition of Cs and MA to FAPbI3 reduces the dispersion in the scaffold, which has a high potential to reduce the migration of iodide and thus improves the structural stability. Additionally, we compare Born effective charges with and without the SOC effect and the DFT-1/2 approach [1]. [1] M. Moaddeli et al, Phys. Chem. Chem. Phys. 25, 25511 (2023).

## HL 56: Heterostructures, Interfaces and Surfaces II

Time: Friday 9:30–11:00 Location: EW 561

HL 56.1 Fri 9:30 EW 561

**Magneto-optical studies of charge transfer excitons in type-II semiconductor quantum wells** — •Johannes Röder[1], Marina Gerhard[1], Cong Ngo[2], Johannes T. Steiner[2], Mikko Wilhelm[1], Christian Fuchs[1], Wolfgang Stolz[1], Stefan W. Koch[1], Torsten Meier[2], Wolfram Heimbrodt[1], and Martin Koch[1] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany — [2]Department of Physics, Paderborn University, Germany

While charge transfer excitons (CTX) are a well-known phenomenon in so called type-II semiconductors, their study with absorption measurements is very challenging, due to the small overlap between the electron and hole wave functions.

This situation was changed by growing 50 asymmetric double quantum wells (ADQWs) via MOVPE, for which earlier studies have already shown a strong CTX absorption. One ADQW consisted of a layer of Ga(As,Sb) and one layer of (Ga,In)As. Among the different samples the Sb-content was varied and a reference sample without the Ga(As,Sb)-layer was grown as well.

The main focus of this presentation is the CTX absorption behavior in a magnetic field. Here we observed the 1s CTXs shift and the formation of higher order excitons in magnetic fields up to 7 T at 1.8 K.

Theoretical calculations via the semiconductor-Bloch equations with a k.p model agree very well with or experimental results, thus confirming our observation of spatially indirect magneto-excitons.

HL 56.2 Fri 9:45 EW 561

**Carbon Nanotubes meet MOF synthesis** — •Marvin J. Dzinnik[1], Necmettin E. Akmaz[1], Adrian Hannebauer[2], Andreas Schaate[2], Peter Behrens[2,3], 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

Metal-organic frameworks (MOFs) are highly porous materials made from metallic ion clusters connected by organic linker molecules. The choice of these building blocks strongly affects the physical and chemical properties like pore size and adsorption behaviour. It has been shown that bringing networks of functionalized carbon nanotubes (CNTs) into a MOF synthesis can lead to a conducting, intergrown hybrid material with chemiresistive sensing properties.[1] We found a method to control UiO-66 MOF growth on individual CNTs. By local pretreatment with an electron beam we can define lines on which MOF growth is inhibited, leaving MOF-free spaces on a particular CNT giving a possible way to fabricate miniaturized MOF/CNT devices and exploring the interaction between these materials.

[1] Schulze, H. A., et al. Electrically Conducting Nanocomposites of Carbon Nanotubes and Metal-Organic Frameworks with Strong Interactions between the two Components. ChemNanoMat, 5(9), (2019), 1159-1169.

HL 56.3 Fri 10:00 EW 561

**Time-resolved unidirectional propagation of exciton-polariton condensates in a Kagome edge mode** — •Christian G. Mayer[1], Tristan H. Harder[1], Philipp Gagel[1], Simon Betzold[1], Monika Emmerling[1], Adriana Wolf[1], Michael D. Fraser[2,3], Sebastian Klembt[1], and Sven Höfling[1] — [1]Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg, Germany — [2]RIKEN Center for Emergent Matter Science Wako-shi, Saitama 351-0198, Japan — [3]Physics & Informatics Laboratories (PHI Lab) NTT Research, Inc. Sunnyvale, CA 94085, USA

Strongly coupled Fabry-Pérot microcavity photons with excitons form hybrid light-matter particles called exciton-polaritons. Surpassing a critical density and inherited by their bosonic statistics, they undergo a phase transition towards a dynamic condensate by stimulated scattering into ground state. Confining the photonic mode in micropillars, an artificial photonic lattice can be created. By implementing this technique, the photonic potential landscape can be shaped to emulate the band structure of a two-dimensional lattice by coupling many pillars.

Here, we utilize a Kagome lattice, in which we observe a site-dependent unidirectional propagation of the polariton condensate along the dense edge due to its intrinsic asymmetric potential. We use a streak camera to time-resolve and visualize the propagation along the edge for multiple lattice sites.

HL 56.4 Fri 10:15 EW 561

**Energy states of excitons in finite-size crystals** — •Pavel Belov[1], Florian Morawetz[1], Sjard Ole Krüger[1], Stefan Scheel[1], Niklas Scheuler[2], Patric Rommel[2], Jörg Main[2], and Harald Giessen[3] — [1]Institut für Physik, Universität Rostock, 18059 Rostock — [2]Institut für Theoretische Physik II, Universität Stuttgart, 70569 Stuttgart — [3]4th Physics Institute and Research Center SCoPE, Universität Stuttgart, 70569 Stuttgart

Due to quantum confinement, electron-hole pairs in finite-size crystals behave rather differently than in bulk materials: in addition to features of the band structure, in the energy spectrum each quantum-confinement subband produces a proper series of Rydberg levels. The

lowest series is attributed to bound electron-hole states, i.e. the exciton states. Moreover, due to the Coulomb coupling of upper subbands to the continuum of lower subbands, electron-hole resonant states appear above the electron-hole scattering threshold. We investigate the dependence of exciton energies on the strength of the quantum confinement. In our study, the energy spectrum of hydrogen-like excitons in $Cu_2O$-based rectangular quantum wells (QWs) is numerically obtained from the solution of the three-dimensional Schrödinger equation. Various crossings and avoided crossings of energy levels as functions of the QW width are observed and categorized based on the symmetry properties of the exciton wave functions. Particular attention is paid to the limiting cases of narrow and wide QWs. Moreover, energies and linewidths of the electron-hole resonant states are obtained by both the stabilization method and the complex scaling technique.

HL 56.5 Fri 10:30 EW 561

**InGaN/GaN nanowires as optical biosensors with dual readout** — •Genrietta Steingelb, Hannah Nell, Rudolfo Hötzel, Stephan Figge und Martin Eickhoff — Universität, Bremen, Deutschland

Due to their specific electrochemical properties, group III-nitrides (III-N) and their nanostructures have been shown to provide an excellent material platform for the application in electrochemical and biochemical sensors [1-4]. Here, we demonstrate that simultaneous dual readout of InGaN/GaN NW arrays by photoluminescence and photocurrent at different bias voltages provides optical biosensors with enhanced selectivity. As examples we demonstrate the detection of pH changes and of the presence of ascorbic acid and discuss the main detection mechanisms of InGaN NWs on GaN NW templates as well as of axial InGaN/GaN NW heterostructures.

[1] G. Steinhoff, M. Hermann, W. J. Schaff, L. F. Eastman, M. Stutzmann and M. Eickhoff, Appl. Phys. Lett. 83, 177 (2003).

[2] F. Ren, S. J. Pearton, Phys. Stat. Sol. (C) 9, 393 (2012).

[3] J. Wallys, J. Teubert, F. Furtmayr, D. M. Hofmann, M. Eickhoff, Nano Lett. 12, 6180 (2012).

[4] M. Riedel, S. Hölzel, P. Hille, J. Schörmann, M. Eickhoff, F. Lisdat, Biosens Bioelectron. 94, 298 (2017).

HL 56.6 Fri 10:45 EW 561

**Properties of higher order Raman modes in confined carbyne** — •Johannes Lechner — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin

Confined carbyne consists of long linear carbon chains (more than 100 atoms) inside carbon nanotubes and is considered a close, stable analogue to the truly 1-dimensional carbon allotrope carbyne. Here we investigate the higher order modes of the Raman active C-mode of single confined carbyne chains by confocal resonant Raman spectroscopy. We observe large frequency shifts which imply strongly anharmonic properties. Analyzing the relative intensities of Raman peaks of different order, we unravel major fluctuations depending on the excitation wavelength, particularly for the second order. Unexpectedly, the relative intensities of different Raman mode orders also change with the frequency of the C-mode. These new discoveries enable further insight into the structural and electronic properties of confined carbyne as a material system.