Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture halls POT/0006, POT/0051, POT/0081, and POT/0251; Poster P1)

Invited Talks

HL 2.1	Mon	9:30–10:00	POT/0051	**Intrinsically stretchable polymers and devices for biosensing applications** — •Ulrike Kraft
HL 2.2	Mon	10:00–10:30	POT/0051	**Complexity in Organic Mixed Ionic Electronic Conductors and its Application in Neuromorphic Computing** — •Hans Kleemann
HL 2.3	Mon	10:30–11:00	POT/0051	**Organic Neuromorphic Interfaces for Biohybrid Systems: Material and Structural Biomimicry of Synaptic Plasticity** — •Francesca Santoro
HL 2.4	Mon	11:15–11:45	POT/0051	**Fully-organic flexible detectors for real-time dose monitoring during radio/proton therapy** — •Beatrice Fraboni
HL 2.5	Mon	11:45–12:15	POT/0051	**Organic LEDs and photodetectors for light-based diagnostics and therapy** — •Caroline Murawski, Rabiul Islam, Siddhartha Saggar, Jens P. Weber
HL 4.1	Mon	9:30–10:00	POT/0251	**X-ray nanodiffraction studies of lead-halide perovskite supercrystals** — Jonas Hiller, Robert Thalwitzer, Ata Bozkurt, Matheus Ferreira, Richard Hodak, Fabian Strauss, Elke Nadler, Gerard Hinsley, Bihan Wang, Kuan Hoon Ngoi, Witold Rudzinski, Ekaterina Kneschaurek, Wojciech Roseker, Michael Sprung, Dmitry Lapkin, Dmitry Baranov, Frank Schreiber, Ivan Vartanyants, Marcus Scheele, •Ivan Zaluzhnyy
HL 11.1	Mon	15:00–15:30	POT/0251	**Quantum Repeater Hardware made from Silicon Carbide** — •Jörg Wrachtrup
HL 11.2	Mon	15:30–16:00	POT/0251	**Diamond based quantum sensing for drug testing** — •Romana Schirhagl
HL 11.3	Mon	16:00–16:30	POT/0251	**The oxygen-related ST1 centre in diamond: a room temperature coherently controllable electron spin** — •Sebastien Pezzagna
HL 11.4	Mon	16:45–17:15	POT/0251	**Silicon quantum emitters emitting in the optical telecommunication range for scalable quantum photonic circuits** — •Yonder Berencén
HL 11.5	Mon	17:15–17:45	POT/0251	**Advances in materials processing for quantum sensing** — •Adam Gali
HL 16.1	Tue	9:30–10:00	POT/0081	**Tailoring the performance of WSe_2 quantum emitters via cavity quantum electrodynamics and coherent driving** — •Ivan Solovev
HL 16.2	Tue	10:00–10:30	POT/0081	**Deterministic single-photon emitters in 2D materials** — •Ursula Wurstbauer
HL 16.3	Tue	10:30–11:00	POT/0081	**Resolving atomic and electronic structure of point defects in MoS_2 by first-principles calculations and scanning tunneling microscopy** — •Hannu-Pekka Komsa
HL 16.4	Tue	11:15–11:45	POT/0081	**Polarization dynamics of isolated defects in hexagonal boron nitride** — Serkan Paçal, Çağlar Samaner, Furkan Ağlarci, Ömer S. Tapşin, •Serkan Ateş
HL 16.5	Tue	11:45–12:15	POT/0081	**Defect-driven quantum emission in 2D materials** — •Magdalena Grzeszczyk

HL 25.1	Wed	9:30–10:00	POT/0251	**Quantum dots for single-electron current sources** — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Niels Ubbelohde, Klaus Pierz, Hans W. Schumacher, Frank Hohls
HL 25.2	Wed	10:00–10:30	POT/0251	**Optical readout of reconfigurable in-plane magnetic domains in CrSBr** — •Aleksandra Łopion, Pierre-Maurice Piel, Manuel Terbeck, Jan-Hendrik Larusch, Jakob Henz, Marie-Christin Heissenbüttel, Thorsten Deilmann, Michael Rohlfing, Zdenek Sofer, Ursula Wurstbauer
HL 25.3	Wed	10:30–11:00	POT/0251	**Ferroelectric switching in Mn-doped epitaxial $BaTiO_3$ films and superlattices on silicon** — •Alfredo Blázquez Martínez, Valentin Väinö Hevelke, Ibukun Olaniyan, Minh-Anh Luong, Ines Häusler, Sven Wiesner, Christoph T. Koch, Dong-Jik Kim, Catherine Dubourdieu
HL 25.4	Wed	11:15–11:45	POT/0251	**Tunability of quantized Hall plateaus** — •Serkan Sirt, Vladimir Umansky, Stefan Ludwig
HL 25.5	Wed	11:45–12:15	POT/0251	**How to achieve high gain in organic photodetectors?** — •Johannes Benduhn
HL 30.1	Wed	15:00–15:30	POT/0081	**Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures** — •Christoph Kastl
HL 42.1	Thu	11:15–11:45	POT/0006	**Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion** — •Verena Streibel, Laura I. Wagner, Elise Sirotti, David A. Egger, Ian D. Sharp
HL 46.3	Thu	15:30–16:00	POT/0051	**Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes** — Somayeh Souri, Katrin Winte, Daniel Lünemann, Daniel Timmer, Elena Mena-Osteritz, Sergei Tretiak, Christoph Lienau, •Antonietta De Sio
HL 49.1	Thu	16:15–16:45	POT/0081	**Phonon-mediated nonlinearity and defects in hexagonal boron nitride** — •Nahid Talebi
HL 53.1	Fri	9:30–10:00	POT/0051	**Organic semiconductors: Opening new perspectives in sustainable electronics** — •Karl Leo

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

See SYFC for the full program of the symposium.

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber, Manuel Meierhofer, Ulrich Höfer
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes

SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — Daniel Lesko, Tobias Weitz, Weizhe Li, Selina Nöcker, Celina Hüttner, Tamara Pröbster, Simon Wittigschlager, Christian Heide, Ofer Neufeld, •Peter Hommelhoff

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

HL 1.1–1.12	Mon	9:30–12:45	POT/0006	**Optical Properties I**
HL 2.1–2.7	Mon	9:30–12:45	POT/0051	**Focus Session: Biocompatible Organic Semiconductors for Artificial Intelligence**
HL 3.1–3.12	Mon	9:30–12:45	POT/0081	**2D Materials I – Excitonic properties**
HL 4.1–4.8	Mon	9:30–12:00	POT/0251	**Perovskite and Photovoltaics: Synthesis and Performance**
HL 5.1–5.7	Mon	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)**
HL 6.1–6.7	Mon	15:00–18:15	HSZ/0003	**Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)**
HL 7.1–7.11	Mon	15:00–17:45	HSZ/0204	**2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)**
HL 8.1–8.12	Mon	15:00–18:15	POT/0006	**Ultra-fast Phenomena I**
HL 9.1–9.6	Mon	15:00–16:30	POT/0051	**Oxide Semiconductors: Growth and Fabrication**
HL 10.1–10.6	Mon	15:00–16:30	POT/0081	**2D Materials II – Electronic and transport properties (joint session HL/TT)**
HL 11.1–11.7	Mon	15:00–18:15	POT/0251	**Focus Session: Quantum Emitters in 3D Semiconductors**
HL 12.1–12.7	Mon	16:45–18:30	POT/0051	**Heterostructures, Interfaces and Surfaces: Photonics**
HL 13.1–13.7	Mon	16:45–18:30	POT/0081	**2D Materials III – Interlayer excitons**
HL 14.1–14.4	Tue	9:30–10:45	HSZ/0105	**Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)**
HL 15.1–15.9	Tue	9:30–12:00	POT/0006	**Organic Semiconductors: Optics and Photonics**
HL 16.1–16.7	Tue	9:30–12:45	POT/0081	**Focus Session: Quantum Emitters in 2D Semiconductors**
HL 17.1–17.10	Tue	9:30–12:15	POT/0251	**Quantum Dots and Wires: Rings, Wires and Transport**
HL 18.1–18.10	Tue	10:00–12:45	POT/0051	**Nanomechanical systems (joint session HL/TT)**
HL 19.1–19.7	Tue	10:30–12:30	HSZ/0201	**Graphene: Growth, structure and substrate interaction (joint session O/HL)**
HL 20.1–20.66	Tue	18:00–20:00	P1	**Poster I**
HL 21.1–21.4	Wed	9:30–10:30	HSZ/0101	**Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)**
HL 22.1–22.6	Wed	9:30–11:00	POT/0006	**Biocompatible Organic Semiconductors**
HL 23.1–23.10	Wed	9:30–12:15	POT/0051	**Transport Properties**
HL 24.1–24.12	Wed	9:30–12:45	POT/0081	**2D Materials IV – Emerging materials and properties**
HL 25.1–25.5	Wed	9:30–12:15	POT/0251	**Focus Session: Young Semiconductor Forum**
HL 26.1–26.56	Wed	9:30–11:30	P1	**Poster II**
HL 27.1–27.8	Wed	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)**
HL 28.1–28.11	Wed	15:00–17:45	HSZ/0401	**Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)**

HL 29.1–29.5	Wed	15:00–16:15	POT/0006	**Quantum Transport and Quantum Hall effects (joint session HL/TT)**
HL 30.1–30.7	Wed	15:00–17:15	POT/0081	**2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)**
HL 31.1–31.5	Wed	15:00–16:15	POT/0251	**Materials and Devices for Quantum Technology I**
HL 32.1–32.9	Wed	15:00–17:30	REC/C213	**2D Materials 2 (joint session DS/HL)**
HL 33.1–33.5	Wed	16:30–17:45	POT/0006	**Nitrides I – Growth and fabrication**
HL 34.1–34.5	Wed	16:30–17:45	POT/0051	**Quantum Dots and Wires: Telecom Wavelength**
HL 35.1–35.9	Wed	16:30–19:00	POT/0251	**Optical Properties II**
HL 36.1–36.4	Wed	17:30–18:30	POT/0081	**2D Materials VI – Optoelectronic properties**
HL 37.1–37.6	Thu	9:30–11:00	POT/0006	**Nitrides II – Designed properties and LED**
HL 38.1–38.12	Thu	9:30–12:45	POT/0051	**Materials and Devices for Quantum Technology II**
HL 39.1–39.11	Thu	9:30–12:30	POT/0081	**2D semiconductors VII – CrSBr and related heterostructures**
HL 40.1–40.11	Thu	9:30–12:30	POT/0251	**Oxide Semiconductors: Transport and Spectroscopy**
HL 41.1–41.7	Thu	11:00–12:45	HSZ/0101	**Quantum Dots and Point Contacts (joint session TT/HL)**
HL 42.1–42.5	Thu	11:15–12:45	POT/0006	**Nitrides III – Emerging thin films and electrochemistry**
HL 43	Thu	13:30–17:00	Infineon	**Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)**
HL 44.1–44.11	Thu	15:00–17:45	HSZ/0204	**2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**
HL 45.1–45.8	Thu	15:00–17:15	POT/0006	**Perovskite and Photovoltaics: Spectroscopy**
HL 46.1–46.7	Thu	15:00–17:15	POT/0051	**Ultra-fast Phenomena II**
HL 47.1–47.4	Thu	15:00–16:00	POT/0081	**2D Materials VIII – Quantum emitters and defects**
HL 48.1–48.8	Thu	15:00–17:15	POT/0251	**Heterostructures, Interfaces and Surfaces: Fabrication and Structure**
HL 49.1–49.4	Thu	16:15–17:30	POT/0081	**Quantum Emitters in 2D Semiconductors**
HL 50	Thu	17:45–19:15	POT/0051	**Members' Assembly**
HL 51.1–51.12	Fri	9:30–12:30	HSZ/0401	**2D Materials: Stacking and heterostructures (joint session O/HL/TT)**
HL 52.1–52.5	Fri	9:30–10:45	POT/0006	**THz and MIR Physics in Semiconductors**
HL 53.1–53.6	Fri	9:30–11:15	POT/0051	**Organic Semiconductors: Carrier Dynamics**
HL 54.1–54.12	Fri	9:30–12:45	POT/0081	**2D Materials IX – Photonic properties and devices**
HL 55.1–55.11	Fri	9:30–12:30	POT/0251	**Quantum Dots and Wires: (Single) Photonics**
HL 56.1–56.5	Fri	11:15–12:30	POT/0006	**Quantum Emitters in 3D Semiconductors**
HL 57.1–57.5	Fri	11:30–12:45	POT/0051	**Nitrides IV – Optical properties**

Members' Assembly of the Semiconductor Physics Division

Thu 17:45–19:15 POT/0051

HL 1: Optical Properties I

Time: Monday 9:30–12:45 Location: POT/0006

HL 1.1 Mon 9:30 POT/0006

Critical-Point Analysis of Ta_3N_5 Light Absorbers from Room-Temperature Photo-Modulated Spectroscopy — •Matthias Quintern[1,2], Johannes Dittloff[1,2], Lukas Wolz[1], Gabriel Grötzner[1,2], Johanna Eichhorn[1], and Ian D. Sharp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, 85748 Garching, Germany — [2]Technical University of Munich, Walter Schottky Institute, 85748 Garching, Germany

Tantalum nitride (Ta_3N_5) thin films are promising photoanode materials for solar water splitting. However, the fundamental nature of the Ta_3N_5 bandgap remains under debate. To overcome the limitations of conventional Tauc-plot analysis, we built a new combined photoreflectance (PR) and phototransmittance (PT) setup. Our measurements indicate a direct fundamental bandgap of 2.1 eV, but also reveal higher-energy critical points. Furthermore, we find that the PR and PT spectra closely match temperature-corrected transient absorption spectra. The overall differences in the transmission spectra are minor, suggesting that the samples share a similar bulk electronic structure. At the same time, the more surface-sensitive PR signals exhibit greater variations and even additional sub-gap features in some samples. By performing measurements using different pump wavelengths and power densities, as well as employing a phase analysis, we assign individual features of PR spectra to a surface layer. This has implications for out-of-plane charge transport properties and interfacial energies, both of which are crucial parameters for photoelectrochemical performance.

HL 1.2 Mon 9:45 POT/0006

OptiMate3B: Three-body-information-based prediction of optical spectra for semiconductors and insulators — •Malte Grunert, Max Grossmann, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Optical spectra of semiconductors and insulators are essential both for many technologically important applications as well as for the understanding of materials. However, their computation via adequate ab initio techniques remains prohibitively expensive for either large-scale studies or many realistic systems. Recently however, machine learning techniques have emerged as promising alternative. We present OptiMate-3B, a line graph attention network capable of predicting the optical spectra of semiconductors and insulators under both the independent particle approximation and the random phase approximation - i.e. incorporating local-field effects - within milliseconds. OptiMate-3B incorporates three-body information to capture angular information in crystalline materials, further enhancing its predictive accuracy. Having been trained on tens of thousands of high-fidelity first-principles spectra, the model generalizes across a broad chemical and structural space. Its open and user-friendly interface facilitates direct integration into high-throughput materials workflows, providing an efficient surrogate for ab initio optical spectroscopy.

HL 1.3 Mon 10:00 POT/0006

Intensity-dependent excitonic second- and third-harmonic generation enhanced by static electric fields — Ruixin Zuo[1], •Matthias Reichelt[1], Cong Ngo[1], Xiaohong Song[2], Weifeng Yang[2,3], and Torsten Meier[1] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Straße 100, D-33098 Paderborn, Germany — [2]School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570288, China — [3]Center for Theoretical Physics, Hainan University, Haikou 570288, China

The many-body Coulomb interaction plays a decisive role in the ultrafast photoinduced carrier dynamics governing semiconductor high-harmonic generation, see, e.g., [1,2]. Moreover, static electric fields were shown to surprisingly enhance excitonic second- and third-harmonic generation [3]. Here, we study this enhancement for material models corresponding to transition-metal dichalcogenides and study the dependencies on several parameters.

[1] A. Trautmann, R. Zuo, G. Wang, W.-R. Hannes, S. Yang, L. H. Thong, C. Ngo, J. T. Steiner, M. Ciappina, M. Reichelt, H. T. Duc, X. Song, W. Yang, and T. Meier, Proc. SPIE **11999**, 1199909 (2022).
[2] J. Hader, J. Neuhaus, J. V. Moloney, and S. W. Koch, Opt. Lett. **48**, 2094 (2023).
[3] R. Zuo, M. Reichelt, C. Ngo, X. Song, W. Yang, and T. Meier, arXiv:2511.05112.

HL 1.4 Mon 10:15 POT/0006

Thin Films of Size-Selected Cu_2ZnSnS_4 and Cu_2NiSnS_4 Nanocrystals: Structural and Optical Properties — •Oleksandra Ivakhno-Tsehelnyk[1], Serhiy Kondratenko[2], Volodymyr Dzhagan[3], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology. — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine. — [3]Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 03038 Kyiv, Ukraine.

An investigation was conducted into thin films of Cu_2NiSnS_4 (CNTS) and Cu_2ZnSnS_4 (CZTS) nanocrystals (NCs) in the context of their promising use for photovoltaics (PV). Colloidal NC ensembles were obtained by "green" colloidal synthesis and directly subjected to size-selective centrifugation, yielding fractions of different sizes. This approach provides a relatively non-toxic and scalable method of producing light-absorbing NC materials. The thin films were prepared by spin-coating the NC fractions onto various substrates. A range of analytical techniques were employed to investigate their properties, encompassing Raman spectroscopy, atomic force microscopy (AFM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and spectroscopic ellipsometry. These techniques enabled the investigation of the relationship between the crystal structure, composition, morphology, and optical properties with the size of CZTS and CNTS nanocrystals.

HL 1.5 Mon 10:30 POT/0006

Simulations of the nonlinear optical dynamics of quantum dot ensembles in a microcavity — •Mohit Kumar[1,2], Hendrik Rose[2], and Torsten Meier[1,2] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany — [2]Institute for Photonic Quantum Systems (PhoQS), Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany

Recently, it has been demonstrated that photon echoes emitted from ensembles of inhomogeneously-broadened quantum dots can be controlled in several ways by suitably designed light pulses [1,2]. The strong coupling of a single two-level system to the mode of a microcavity results in a complex nonlinear optical dynamics [3]. Here, we present numerical simulations of the coherent dynamics of quantum dots ensembles, described as two-level systems, inside a single-mode microcavity. The coupling to the field mode results in a complex dynamics which is studied numerically as function of the relevant system parameters and for different excitation conditions.

[1] A. N. Kosarev, H. Rose, S. V. Poltavtsev, M. Reichelt, C. Schneider, M. Kamp, S. Höfling, M. Bayer, T. Meier, and I. A. Akimov, Comm. Physics **3**, 228 (2020).
[2] S. Grisard, A. V. Trifonov, H. Rose, R. Reichhardt, M. Reichelt, C. Schneider, M. Kamp, S. Höfling, M. Bayer, T. Meier, and I. A. Akimov, ACS Photonics **10**, 3161 (2023).
[3] M. Koch, J. Shah, and T. Meier, Phys. Rev. B **57**, R2049(R) (1998).

HL 1.6 Mon 10:45 POT/0006

Optical Limiting Induced by Excited-State Absorption in Thiophene Oligomers — •Mustapha Driouech, Michele Guerrini, and Caterina Cocchi — Friedrich-Schiller Universität Jena, Institute for Condensed Matter Theory and Optics, 07743 Jena, Germany

Optical limiting (OL) is a nonlinear effect that reduces light transmission at high intensities, providing protection for sensitive optical devices and human eyes. Non-perturbative ab initio methods have proven to be powerful predictive tools for OL [1]. In this work, we investigate the optical absorption spectra of a set of thiophene oligomers under the influence of a broadband, instantaneous electric field [2]. At sufficiently high intensities, absorption peaks that are absent in the linear response emerge below the absorption onset in the linear regime. To elucidate the optical nonlinearities involved, we perform pump-probe

simulations and analyze the population dynamics, revealing that these emergent features originate from excited-state absorption in the near-infrared to visible region. Further analysis, taking into account both molecular length and applied laser intensity, demonstrates how these factors influence the nonlinear response. Our results show that this fully ab initio approach can accurately capture and unravel the fundamental processes driving optical nonlinearities in thiophene oligomers.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).
[2] M. Driouech, et al., J. Phys. Chem. Lett 16, 11867 (2025).

15 min. break

HL 1.7 Mon 11:15 POT/0006

Polarization-resolved Raman measurements on optically anisotropic crystals — •Susanne Moritz, Lukas Trefflich, Ron Hildebrandt, Marius Grundmann, and Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Raman spectroscopy provides a powerful, non-destructive way to probe lattice vibrations, crystal symmetry, and electron-phonon interactions. For years, optically anisotropic materials have been gaining importance in solid-state physics research. These materials are investigated by measuring the Raman intensity in two configurations, namely cross-polarized and parallel polarization. However, due to their low symmetry, this is not sufficient in order to extract the properties of the Raman tensor and extensive polarization-resolved Raman measurements are required for a precise determination, particularly of the Raman tensor [1,2,3]. Here, we present an efficient measurement scheme in order to determine the Raman tensor of optically anisotropic materials with high precision. Special care must be taken regarding the influence of the used polarizing optics, such as half-wave plates, as well as the impact of the non-idealities of all optical elements included in the setup, such as mirrors or beam splitters. For this purpose, we also show a procedure for calibrating these elements.

[1] C. Kranert et al., Phys. Rev. Lett. **116**, 127401 (2016)
[2] C. Kranert et al., Sci. Rep. **6**, 35964 (2016)
[3] R. Hildebrandt et al., Appl. Phys. Lett. **119**, 121109 (2021)

HL 1.8 Mon 11:30 POT/0006

Quadrupole Transitions in Molecules from Real-Time Time-Dependent Density Function Theory — •Anvar Khujakulov[1], Michele Michele Guerrini[1], Carlo Andrea Rozzi[1], and Caterina Cocchi[2] — [1]Institute for Condensed Matter Theory and Optics, 07743 Jena, Germany — [2]Istituto Nanoscienze - 41125 Modena, Italy

The breakdown of the dipole approximation in tightly focused or short-wavelength laser fields is driven by spatial electric field variations, leading to significant beyond-dipole effects including quadrupole transitions and a nonlinear optical response [1]. We extend the Yabana-Bertsch implementation of real-time time-dependent density functional theory to include quadrupole transitions in the absorption cross-sections and apply the developed approach to atoms and small molecules. Our results reveal absorption peaks appearing above the linear absorption onset, a clear signature of quadrupole transitions. Critically, for molecules with appropriate symmetry, the quadrupole contribution to the absorption cross-section is maximized when a specific molecular axis aligns with the electric field gradient, analogous to the dipole case. By systematically rotating the molecular axis relative to the laser polarization vector, we calculate the orientation-dependent absorption cross-section and differentiate the contributions from dipole and quadrupole transitions. We quantitatively demonstrate that quadrupole transition is not a minor effect but a significant contributor to absorption spectra beyond the dipole approximation.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).

HL 1.9 Mon 11:45 POT/0006

Phase-matched electron-photon interactions enabled by 3D printed helical waveguides — •Masoud Taleb[1], Mohsen Samadi[2], and Nahid Talebi[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Department of Electrical and Information Engineering, Kiel University, 24143 Kiel, Germany

We demonstrate a new phase-matching mechanism between free electrons and guided optical modes using 3D-printed helical waveguides. The structure consists of a polymer micro-fiber coated with a thin gold layer, fabricated by two-photon polymerization. When an electron beam propagates parallel to the helix axis, the helical geometry extends the optical path and enables sequential, phase-synchronous coupling to a plasmonic hybrid mode. This interaction unifies elements of Smith-Purcell and Cherenkov emission and yields a strong, highly directional visible-light output. Cathodoluminescence measurements reveal a dominant emission near 2.1-2.2 eV, collimated along the electron trajectory and exhibiting circular polarization dictated by the helix handedness. The observed photon yield (~0.02 photons per electron for an 11-turn helix) exceeds that of planar electron-driven photon sources by more than two orders of magnitude. These results introduce helical micro-waveguides as an efficient platform for directional, polarization-controlled electron-photon interactions.

HL 1.10 Mon 12:00 POT/0006

Quantum-engineered CaAlSiN3 via terbium substitution: coupling spin, optical, and lattice responses in a rare-earth nitride host — •Sikander Azam and Jan Minar — University of West Bohemia New Technologies - Research Centre Univerzitní 8 301 00 Plzeň Czech Republic

Rare-earth nitrides attract interest because they link optical activity, magnetism, and mechanical stability. CaAlSiN3 is a robust wide-gap host, but the microscopic role of terbium substitution is not well established. We study pristine and Tb-doped CaAlSiN3 (8.5 and 17 percent) using spin-polarized density functional theory within GGA+U and spin-orbit coupling in WIEN2k. Tb narrows the bandgap and introduces 4f-derived mid-gap states that enhance visible-range absorption. The densities of states show hybridization between Tb 4f levels and the surrounding network. The optical response shows higher absorption, a larger refractive index, and shifts in dielectric features that follow these electronic changes. Simulated Tb L*-edge X-ray absorption spectra display white-line shifts and peak broadening with increasing Tb content, consistent with the modified unoccupied 4f states. Tb carries a strong local moment, raising the total moment to about 11.8 μB at higher doping. All compositions remain mechanically stable, and bulk and shear moduli increase moderately. The piezoelectric response also strengthens, with d33 and e33 roughly doubling compared to the undoped host. These results show that Tb substitution tunes the electronic, magnetic, optical, and mechanical behaviour of CaAlSiN*, supporting its potential in photonic and spin-related applications.

HL 1.11 Mon 12:15 POT/0006

Accurate computation of Berry connection purely limited by basis set completeness — Martin Thümmler[1], •Alexander Croy[1], Thomas Lettau[2], Ulf Peschel[2,3], and Stefanie Gräfe[1,3,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena — [3]Abbe School of Photonics, Friedrich Schiller University Jena — [4]Fraunhofer Institute for Applied Optics and Precision Engeneering Jena

Wannierization provides a reliable framework for interpolating operator matrix elements in the Brillouin zone. This Fourier-type interpolation of the matrix elements of **k**-local operators, e.g., the Hamiltonian, is well understood. However, the Berry connection is computed from the overlap matrices of the cell periodic parts of the Bloch functions with different **k** and hence non-local. So far, all proposed interpolation schemes do not account for the matrix structure of the overlap matrices, but treat the matrix elements as independent when computing the Berry connection. In this work, we propose a consistent interpolation scheme based on the matrix logarithm. Its accuracy is only limited by the basis set incompleteness of the considered bands in the ab-initio calculation. The quality of the new interpolation scheme is demonstrated by an improved agreement between the velocity and momentum operator over the full Brillouin zone. As an application, we demonstrate how this refinement impacts the predicted linear and non-linear optical properties of semiconductors.

HL 1.12 Mon 12:30 POT/0006

Focused Ion Beam (FIB) patterned Microcavities for Topological Lasers — •Lorenz Löffler[1,4], Dominik Horneber[1,4], Jakob Lindenthal[2,4], Johannes Düreth[1,4], Markas Sudzius[2,4], Monika Emmerling[1], Martin Kamp[3], Simon Betzold[1,4], Johannes Benduhn[2,4], Sven Höfling[1,4], Karl Leo[2,4], and Sebastian Klembt[1,4] — [1]University of Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), and Institute of Applied Physics, Technische Universität Dresden — [3]University of Würzburg, Physikalisches Institut and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems — [4]Würzburg-Dresden Cluster of Excellence ct.qmat

Topological lasers can be realized by coupling individual photonic resonators in topologically non-trivial lattice geometries. Optical microcavities have been found to be a promising platform for studying topological laser interfaces with long-range coherence. The fabrication of such structures typically involves etching of the microcavity and through the emitter layer. In our work, we create the photonic potential by FIB milling of a glass substrate prior to depositing dielectric Bragg reflectors. This technique allows the potential to be engineered while keeping the emitter layer intact. Here, the emitter is either semiconductor quantum wells or the organic semiconductor Alq_3 doped with DCM dye. By exploring modified lattice geometries that enhance the interface-to-bulk ratio as well as temperature-dependent studies, we aim for the next step towards practical topological lasers.

HL 2: Focus Session: Biocompatible Organic Semiconductors for Artificial Intelligence

This Focus Session deals with electronic components that interface with biological systems and offer diverse possibilities in research and applications, e.g., in healthcare. Carbon-based organic semiconductors are particularly well-suited to this interface: They enable electronic devices with a broad spectrum of electronic and optoelectronic functions that are biocompatible and often even resorbable by the body. Furthermore, they are particularly well-suited for neuromorphic functions that enable local data analysis computing towards artificial and neurohybrid intelligence. Turning this vision into practice requires extensive interdisciplinary research on semiconductor materials, components, and electronic systems. This Focus Session aims to provide an overview of the current state of the art including new organic materials, devices and core applications in bioelectronic interfaces.

Organized by Karl Leo

Time: Monday 9:30–12:45 Location: POT/0051

Invited Talk HL 2.1 Mon 9:30 POT/0051
Intrinsically stretchable polymers and devices for biosensing applications — •Ulrike Kraft — Organic Bioelectronics Research Group, MPI for Polymer Research, Mainz, Germany

Organic electrochemical transistors (OECTs) currently attract vast interest for biosensing applications due to their, intrinsic signal amplification and low operating voltages, enabling sensing in close contact to the human body and in aqueous environments with liquid analytes. Furthermore, the low elastic modulus of polymers can be tailored to match that of soft biological tissues, drawing increasing interest towards soft and stretchable health-monitoring devices.

The first part of the talk will focus on our work on biosensors based on planar OECTs that are functionalized with antibodies for e.g. the detection of the SARS-CoV-2 spike protein or with aptamers for the detection of e.g. cytokines, which are proteins crucial for immune regulation and inflammatory responses.

In the second part, I will summarize our efforts on stretchable electronics including a fast and reliable transfer-printing method for the deposition of conductive polymer films (e.g. PEDOT:PSS) onto stretchable, biodegradable substrates Taking advantage of this method and infusing the substrates with small-molecule plasticizers that also diffuse into the conductive films, improves the electrical performance as well as the mechanical properties. Lastly, this platform is employed for studying the effect of strain on the figures-of-merit of intrinsically stretchable OECTs.

Invited Talk HL 2.2 Mon 10:00 POT/0051
Complexity in Organic Mixed Ionic Electronic Conductors and its Application in Neuromorphic Computing — •Hans Kleemann — Technische Universität Dresden, Dresden, Germany

Complexity is decisive property enabling systems to work at the edge of chaos, which is necessary for resource-efficient computing and the design of intelligent machines. The complex behavior of a system originates from the nonlinear properties of all its components, resulting in a plethora of different signatures such as multi-state stability, stochastic oscillations, etc. These nonlinear properties and their couplings need to be understood and modeled to develop intelligent & energy-efficient computers.

Organic mixed ionic-electronic conductors (OMIECs) based on conjugated polymers open up a fascinating field of research where the ionic-electronic coupling, in combination with correlation effects at high charge carrier densities enables the implementation of various paradigms of neuromorphic computing. In this contribution, I will discuss the various signatures of nonlinearity and complexity that have been observed in OMIECs in recent years and review the current understanding of these effects. Furthermore, I will discuss how phenomena such as hysteresis and bistability can be employed to design fundamental elements of asynchronous computing, such as spiking neurons or C-elements, providing the foundation for the efficient implementation of approaches of stochastic computing in hardware. Finally, I will present a technology platform that allows us to integrate such devices in all-printed, complementary circuits operating above 1kHz.

Invited Talk HL 2.3 Mon 10:30 POT/0051
Organic Neuromorphic Interfaces for Biohybrid Systems: Material and Structural Biomimicry of Synaptic Plasticity — •Francesca Santoro — Forschngszentrum Jülich

Organic neuromorphic interfaces offer a promising route toward biohybrid systems that emulate neural function. We present PEDOT:PSS-based organic electrochemical transistors that exploit mixed ionic*electronic conduction and biocompatibility to reproduce key mechanisms of synaptic plasticity. Through the integration of biogels and azopolymer-functionalized conjugated polymers, neural activity is modulated by chemical and optical stimuli, enabling short- and long-term plasticity and interactions with neurotransmitters such as dopamine and glutamate. Beyond planar devices, 2.5D and 3D microfabricated organic semiconductor architectures fabricated by two-photon lithography or electrodeposition mimic neuronal morphology and promote cell adhesion and connectivity. The mechanical compliance of these materials supports stable interfacing with soft tissues, underscoring the role of material and structural biomimicry in next-generation organic biohybrid neuromorphic platforms.

15 min. break

Invited Talk HL 2.4 Mon 11:15 POT/0051
Fully-organic flexible detectors for real-time dose monitoring during radio/proton therapy — •Beatrice Fraboni — Department of Physics and Astronomy , University of Bologna, Italy

The development of detectors for high energy ionizing radiation is a long-lasting research topic not only for fundamental applications but also for medical applications in radio and hadron therapy. Innovative sensors are needed, able to provide, in-situ and in real-time, an accurate recording and mapping of the dose delivered during a treatment plan. Organic small molecules and polymers are promising active layers for advanced dosimetry purposes, as their mechanical features allow the development of devices able to adapt to complex contoured surfaces with outstanding portability (low power operation) and lightweight. They also provide the unique possibility to develop human-tissue-equivalent dosimeters, thanks to their density and composition. The physical process of radiation detection for organic thin-film based detectors will be discussed in two different configurations: 1) the direct one, based on a simple planar device with an organic thin film as active conversion layer, and 2) the indirect one, based on a polysiloxane-based scintillating layer effectively coupled to an organic phototransistor (OPT). A new kinetic model has been developed to describe the organic dosimeter response mechanism under photon/proton irradiation and to provide further insight into the physical processes

controlling its response.

I.Fratelli et al Science Advances 11, 7633 (2025) S. Calvi et al., NPJ Flexible Electronics 7,5 (2023)

Invited Talk HL 2.5 Mon 11:45 POT/0051

Organic LEDs and photodetectors for light-based diagnostics and therapy — •Caroline Murawski[1,2], Rabiul Islam[1,2], Siddhartha Saggar[1,2], and Jens P. Weber[1,2] — [1]Institute of Solid-State Electronics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, 04736 Waldheim, Germany

Light-based biomedical sensing and therapy enables highly precise, timely and contactless interventions and range from neuronal stimulation via optogenetics over sensing cellular activity by functional fluorescence to monitoring health signals using wearable devices. Organic semiconductors are ideally suited building blocks due to their tunability of material properties, mechanical flexibility and ability for patterning to microscopic shapes. Here, I will present the development of organic LEDs (OLEDs) and photodiodes (OPDs) as light sources and sensors for biomedical applications. The OLEDs are tailored towards high power output and application-specific angular and spectral emission properties. Devices are fabricated on flexible substrates, patterned to sub-mm scale, and applied in optogenetics and fluorescence imaging. Furthermore, I will show flexible OPDs used for photoplethysmography at ambient light conditions and under water.

HL 2.6 Mon 12:15 POT/0051

Reservoir computing with mixed ionic-electronic conductors — •Richard Kantelberg, Hans Kleemann, and Karl Leo — Institut für Angewandte Physik, TU Dresden

Reservoir computing (RC) is a promising paradigm for machine learning that utilizes dynamic systems, termed as reservoirs, to process and analyze complex temporal data. Organic mixed ionic electronic conductors (OMIECs) have emerged as a novel class of materials with intriguing properties, such as their ability to exhibit both electronic and ionic conductivity, as well as their biocompatibility, flexibility, and low power consumption[1]. These features make OMIECs particularly suitable for the development of unconventional computing architectures in the field of bioelectronics[2]. We present recent findings interlinking electronic conductivity, system nonlinearity and reservoir size with the neuromorphic functionality and RC performance of self-organized and structured OMIEC reservoirs. This study includes novel insights into the differences and similarities of p-type, n-type and ambipolar semiconductors in terms of operation speed and energy consumption. The recent progress in reservoir computing using organic mixed ionic electronic provides valuable knowledge for the targeted development OMIEC reservoirs.

References 1.*Paulsen, B. D., Tybrandt, K., Stavrinidou, E. & Rivnay, J. Organic mixed ionic*electronic conductors. Nat. Mater. 19, 13*26 (2020). 2.*van de Burgt, Y., Melianas, A., Keene, S. T., Malliaras, G. & Salleo, A. Organic electronics for neuromorphic computing. Nat. Electron. 1, 386*397 (2018).

HL 2.7 Mon 12:30 POT/0051

Redundant information in physical reservoir computing — •Andreas Hofacker, Richard Kantelberg, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (DC-IAPP), TU Dresden, Dresden, Germany

Maximizing the processing power of a physical reservoir given its physical constraints is crucial for practical applications, but remains an open problem. As a basis for such an optimization, a quantity measuring reservoir capability is needed. To address this need, we propose the use of independent component analysis for assessing information content in reservoir outputs. We present evaluations of organic mixed ionic-electronic conductor based physical and simulated reservoirs and show that task-specific performance is linked to information redundancy in the output channels. By leveraging this insight, sparser reservoir readout can be realised without loss of performance.

HL 3: 2D Materials I – Excitonic properties

Time: Monday 9:30–12:45 Location: POT/0081

HL 3.1 Mon 9:30 POT/0081

Exciton-Electron Complexes in Multilayer Transition-Metal Dichalcogenides — •Florian Hirsch[1], Alexandra Hübler[1], Jonas von Milczewski[2], and Richard Schmidt[1] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

Understanding few-body correlations in van der Waals heterostructures is essential for uncovering emergent electronic phases in layered quantum materials. We report recent progress in identifying exciton-electron-electron bound states in multilayer transition-metal dichalcogenides (TMDs). Starting from the two-body problem, we employ complementary theoretical approaches to characterize bound states and systematically extend this framework to the four-body regime. Within an effective-mass model, we solve the resulting few-body Hamiltonians using exact diagonalization, enabling efficient exploration of material and geometric parameters. This allows us to map out regimes in which such exciton-electron complexes become bound. Our results provide a versatile framework for investigating exciton-mediated correlations in complex multilayer TMD structures and related systems, including platforms where exciton-induced electron pairing or superconductivity may emerge.

HL 3.2 Mon 9:45 POT/0081

Intra- and Interlayer Excitons in TMDC bilayers under external influence — •Jan-Hauke Graalmann and Michael Rohlfing — University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

External influences lead to several changes in the optical spectrum of TMDC bilayers obtained by solving the Bethe-Salpeter. We discuss both the effect of applied pressure and that of an electric field [1,2].

To get the deformation induced by applied pressure, we use Hooke's law. In this case, our investigations show an effective shift of the intralayer A exciton whose direction depends on the stress conditions and we observe a similar behavior for the interlayer exciton, while the shift rate is smaller for the latter. Our results for the 2H-MoS_2 bilayer compare very well with available room-temperature measurements for the interlayer exciton.

An electric field applied perpendicular to the 2H-$MoSe_2$ bilayer does not lead to a deformation, but instead to a Stark shift of the excitons. To explain that, we focus on the lifting of the degeneracy in the band structure by breaking the symmetry of the potential.

[1] P. Steeger, J. Graalmann et al., nano Lett., 23, (2023)
[2] J. Jasiński et al., Nat Commun 16, 1382, (2025)

HL 3.3 Mon 10:00 POT/0081

Optical probing of the gate-tunable electronic band structure of bilayer graphene using a WSe_2 sensor layer — •Jonas Blum[1], David Tebbe[1], Takashi Taniguchi[2], Kenji Watanabe[2], Lutz Waldecker[1], Christoph Stampfer[1,3], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]National Institute for Materials Science, Namiki, Tsukuba, Japan — [3]PGI-9, Forschungszentrum Jülich, Jülich, Germany

Rydberg excitons in transition-metal dichalcogenide monolayers are highly sensitive to their dielectric environment. Previous work has shown that reflection-contrast spectroscopy provides a non-invasive optical probe of their binding energies, enabling the detection of subtle variations in the charge-carrier density n in adjacent layers of van der Waals (vdW) heterostructures. Here, we apply this technique to a fully hBN-encapsulated WSe_2/bilayer-graphene (BLG) device with graphite top and bottom gates and compare the optical response with transport measurements. By applying a displacement field D, we open a band gap in BLG. As the Fermi level is tuned from the valence band across the band gap into the conduction band, we capture changes in n through shifts in the 2s exciton binding energy. These measurements further allow us to resolve the layer population of BLG upon sign reversal of D. We also demonstrate optical quantum Hall measurements, enabling extraction of gate lever arms optically. Unlike transport measurements, this optical technique offers highly local, spatially-resolved access to the electronic band structure of BLG.

HL 3.4 Mon 10:15 POT/0081

Anisotropic Excitonic Response in $MoSe_2$-WSe_2 Lateral Heterostructures — •Miguel Morales Cocera[1,2], Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

We investigate lateral heterostructures of transition-metal dichalcogenide monolayers, in particular $MoSe_2$-WSe_2. In these systems, the one-dimensional (1D) interface together with the type-II band alignment enables the emergence of 1D exciton physics within a two-dimensional monolayer material, with the "inter-layer" excitons retaining near monolayer-level brightness. Motivated by the recent experimental observation of these spatially indirect excitons [1], we calculate the exciton and trion fine structure using ab initio many-body screened configuration interaction [2]. We find that the lowest bright exciton state is non-degenerate due to the loss of symmetry induced by the 1D interface. Moreover, the many-body dipoles of these two excitons lie along different in-plane polarization axes, leading to an anisotropic optical response that may be useful for optoelectronic applications.

[1] R. Rosati, et al., Nat. Commun. 14, 2438 (2023)
[2] Mørch Nielsen, C.E., Fischer, F. & Bester, G. npj 2D Mater. Appl. 9, 11 (2025)

HL 3.5 Mon 10:30 POT/0081

Substrate interaction on local exciton/trion ratio in mono- to few-layer WS2 — •Appanna Parvangada[1,2], Dmitrii Sychev[1], and Ilka Hermes[1] — [1]Leibniz Institute of Polymer Research Dresden e.V., Dresden, Germany — [2]Institute of Applied Physics, Dresden University of Technology, Dresden, Germany

Two-dimensional Tungsten Disulfide (WS2) possesses distinctive optoelectronic properties such as high photoluminescence yield, a tunable band gap, large exciton binding, quantum confinement, strong-light matter interaction. The combination with low dimensionality makes them a favorable candidate for a variety of lightweight and flexible optoelectronic devices such as photodetectors, solar cells and LEDs.

However, large-scale industrial implementation of optoelectronic 2D materials is often impeded by their high spatial heterogeneity, caused by nanoscale variations in layer thickness, substrates interactions and local strain. Thus, standard optical characterization methods like Photoluminescence (PL) and Raman spectroscopy, which commonly provide such information, can lack the spatial resolution to resolve these variations. Here, electrical atomic force microscopy (AFM) methods with in-situ illumination at different wavelengths deliver nanoscale information on the impact of layer thickness, changes in substrates interactions and local strain onto the material's optoelectronic response.

In our study, we demonstrate the capability of photo-Kelvin probe force microscopy (pKPFM) to capture local photo-potential in mono- and few-layer WS2 and correlate PL spectroscopy. Furthermore, we investigate the impact of substrates on the local charge carriers.

HL 3.6 Mon 10:45 POT/0081

Signatures of efficient intervalley scattering by acoustic phonons in WSe2 monolayers — •Hendrik Lambers[1], Daniel Groll[2], Daniel Wigger[2], Nihit Saigal[1], Lara Blinov[1], Tilmann Kuhn[2], Alexander W. Holleitner[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster — [2]Institute of Solid State Theory, University of Münster — [3]Walter Schottky Institute, Technical University of Munich

When group VI TMDC are thinned down to the monolayer limit, their bandgap transfers from indirect to direct. While their strong exciton dominated light-matter coupling can be easily investigated by optical spectroscopy, exciton-phonon coupling is often inaccessible, even though it is important for exciton thermalization and intervalley scattering. We employ resonant Raman scattering at cryogenic temperatures to study the exciton phonon coupling in WSe_2 monolayers. In resonance with the WSe_2 exciton, we observe rich Raman spectra. Here, we focus on the resonance profiles of the degenerated A_1'/E' mode, that exhibits two asymmetric resonance peaks that cannot be described by a first order Raman scattering process. A higher-order Raman scattering process including simultaneous generation and annihilation of acoustic M-point phonons describes the experimental resonance profile well. Our results indicate a strong electron phonon coupling and efficient intervalley scattering between the nearly degenerate direct and indirect exciton transitions in WSe_2. The findings are relevant to understand unusual bright emission in WSe_2 monolayers despite spin-forbidden lowest interband transition.

15 min. break

HL 3.7 Mon 11:15 POT/0081

Transport of exciton complexes in the presence of Fermi sea of free carriers in monolayer semiconductors — •Minushree Rout[1], Koloman Wagner[1,2], Jonas Ziegler[1,2], Raul Perea-Causin[3], Samuel Brem[4], Ermin Malic[4], and Alexey Chernikov[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Department of Physics, University of Regensburg, Germany — [3]Department of Physics, Stockholm University, Sweden — [4]Department of Physics, Philipps-Universität Marburg, Germany

Exciton-carrier interactions in doped monolayer semiconductors present an interesting and technologically relevant scenario in solid-state physics. Among the consequences is the formation of trions-three particle system formed when excitons bind with free charge carriers. Here, we aim to explore how trion-phonon and exciton-carrier interactions influence excitonic quasiparticle diffusion using transient microscopy. Theoretical results predict that trions have reduced mobility at low carrier densities due to strong phonon coupling and increased mass. At higher densities, effective trion diffusion should increase significantly due to the Fermi pressure effect. Previous experimental studies revealed that exciton diffusion shows a non-monotonic dependence on carrier density, transitioning from elastic scattering regime to the formation of bound quasiparticle states like trions and fermi-polarons. This work aims to uncover the fundamental mechanisms governing the transport of light-emitting quasiparticles in the presence Fermi-bose mixtures in 2D semiconductors and experimentally test the prediction of the Fermi-pressure effect.

HL 3.8 Mon 11:30 POT/0081

Investigation of dynamics and character of excitons in WSe_2 and $MoSe_2$ multilayers — •Anna Weindl[1], Matthias Brem[1], Jennifer Lehner[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan

We report about our time-resolved Faraday ellipticity (TRFE) experiments on multilayers of the transition metal dichalcogenide WSe_2 and $MoSe_2$. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the pseudospin oscillations that appear in the TRFE signal when we apply an in-plane magnetic field to our multilayer samples. Now we try to characterize and manipulate these oscillations by playing with different experimental parameters. Varying the angle of the magnetic field, adding an electric field or investigating the layer dependence are examples for our toolbox of parameters to gain further insights into the dynamics of the multilayers. The current results, for example on the resonance behavior of the oscillations and the layer-dependent starting point of the oscillations, will be presented.

[1] S. Raiber *et al.*, Ultrafast pseudospin quantum beats in multilayer WSe_2 and $MoSe_2$, Nat. Commun. 13, 4997 (2022).

HL 3.9 Mon 11:45 POT/0081

In-situ mapping of pressure-induced exciton traps in suspended MoS2 monolayers using Fabry-Perot interference — •Niklas Walter[1,3], Leonard Geilen[1,3], Lukas Schleicher[2,3], Alexander Musta[1,3], Anne Rodriguez[3], Benedict Brouwer[1,3], Eva Weig[2,3], and Alexander Holleitner[1,3] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Chair of Nano and Quantum Sensors, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

We demonstrate the in-situ readout of the spatial profile of suspended MoS2 monolayers hosted on substrates with nanostructured holes. As the profiles are spatially bent, the suspended MoS2 monolayers act as exciton traps with a tunable luminescence intensity and energy. The tunability is realized by controlling the environmental pressure on the monolayers, which allows one to control hundreds of suspended MoS2 monolayers on a single substrate. The in-situ readout is based on Fabry-Perot interferences and a model of the corresponding reflectance

contrast maps of the investigated monolayers.

HL 3.10 Mon 12:00 POT/0081

Coherent two-dimensional electronic spectroscopy integrated with confocal microscopy for probing 2D materials — •Trideep Kawde, Pavel Trofimov, Matteo Russo, Anton Trenczek, and Hélène Seiler — Freie Universität Berlin, 14195, Berlin, Germany

Two-dimensional electronic spectroscopy is a powerful tool for probing ultrafast processes in van der Waals materials and heterostructures. As these structures are typically only 10x100 μm in size and highly heterogeneous, the challenge of ultrafast studies on such materials is to balance requirements in spatial and angular resolutions - often requiring highly dispersive microscope objectives - with temporal resolution. We present a coherent 2D electronic spectroscopy setup integrated with a confocal back focal plane imaging setup, featuring high magnification, spatial and angle resolution, while maintaining a time resolution of ∼15 femtosecond. We demonstrate this approach on an exfoliated WSe_2 monolayer. The data reveal <100 femtosecond homogeneous linewidth broadening of the A exciton lineshape, indicating rapid exciton-energy fluctuations. These measurements provide insight into dephasing mechanisms such as excitation-induced dephasing, which sets fundamental limits to coherent control and quantum-optical applications.

HL 3.11 Mon 12:15 POT/0081

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

With wavelengths in the micrometer range at GHz frequencies, surface acoustic waves (SAWs) are a versatile tool for radio frequency control and probing of charge carrier dynamics in novel semiconductor nanostructures. They are generated on a piezoelectric chip and routed over long distances to couple either mechanically or electrically to many solid-state nanosystems [1]. In our experiments, we fabricated hybrid lithium niobate SAW-devices in which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials were transferred. We investigated the influence of SAW-induced dynamic electric and strain fields on the photoluminescence (PL) of various TMDCs and their heterostructures. By combining optical and acoustic measurements, we were able to gain insights on the charge carrier dynamics and their resulting impact on exciton recombination and lifetime [2].

[1] Per Delsing et al 2019, J. Phys. D: Appl. Phys. 52 353001 [2] Emeline Nysten et al 2024, Adv Mater 36 e2402799

HL 3.12 Mon 12:30 POT/0081

Dark exciton activation in WSe_2 monolayer by tip-enhanced photoluminescence spectroscopy — Adlen Smiri, Fenda Rizky Pratama, and •Takeshi Nakanishi — MathAM-OIL AIST, Sendai, Japan

Dark excitons in 2D transition metal dichalcogenide semiconductors are characterized by long lifetimes, making them highly attractive candidates for quantum computing and optoelectronics.The purpose of this paper is to theoretically address the interactions between local electromagnetic fields and dark excitonic states, and show that the strong out-of-plane near field from a metallic tip enhances radiative recombination of spin-forbidden dark excitons by providing additional in-plane momentum to overcome momentum mismatch [1]. Using ab initio calculations, a Wannier-Mott exciton model, and a numerical solution of the Laplace equation, we model the tip-enhanced near-field and its interaction with excitons via first-order time-dependent perturbation theory. Focusing on WSe_2 monolayers, we demonstrate that the activation of dark excitons is attributed to the strong z-component of the near field induced by the tip. We also analyze substrate screening effects on excitonic properties and lifetimes. Our results offer a theoretical framework for controlled activation of dark excitons toward quantum and nanophotonic applications.

[1] Adlen Smiri, F. R. Pratama and Takeshi Nakanish, npj 2D Materials and Applications 9, 88 (2025)

HL 4: Perovskite and Photovoltaics: Synthesis and Performance

Time: Monday 9:30–12:00 Location: POT/0251

Invited Talk HL 4.1 Mon 9:30 POT/0251

X-ray nanodiffraction studies of lead-halide perovskite supercrystals — Jonas Hiller[1], Robert Thalwitzer[1], Ata Bozkurt[1], Matheus Ferreira[2], Richard Hodak[1], Fabian Strauss[1], Elke Nadler[1], Gerard Hinsley[3], Bihan Wang[3], Kuan Hoon Ngoi[3], Witold Rudzinski[4], Ekaterina Kneschaurek[1], Wojciech Roseker[3], Michael Sprung[3], Dmitry Lapkin[1], Dmitry Baranov[2], Frank Schreiber[1], Ivan Vartanyants[3], Marcus Scheele[1], and •Ivan Zaluzhnyy[1] — [1]University of Tübingen — [2]Lund University — [3]Deutsches Elektronen-Synchrotron DESY — [4]University of Krakow

We synthesize mechanically robust supercrystals built from cubic lead halide perovskite nanocrystals by a two-layer phase diffusion self-assembly with acetonitrile as the antisolvent. This method yields highly faceted thick supercrystals, which are robust enough to be picked up and relocated by microgrippers. We employed X-ray nanodiffraction together with high-resolution scanning electron microscopy and atomic force microscopy to reveal the structure of $CsPbBr_3$, $CsPbBr_2Cl$, and $CsPbCl_3$ supercrystals and explain their unusual mechanical robustness. We show that the removal of organic ligands from perovskite nanocrystals results in a size gradient of the nanocrystals within the supercrystals.

Hiller et al., ACS Nano **19** (2025) 26117

HL 4.2 Mon 10:00 POT/0251

Impact of Antisolvents on Halide Perovskite Nanocrystal Synthesis — •Tim Julius Hashagen, Leo Luber, and Alexander Skyrme Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Lead halide perovskite nanocrystals (NCs) offer highly tunable optical properties and high photoluminescence efficiencies, making them promising for optoelectronic and photocatalytic applications. Their synthesis, however, is extremely sensitive to the choice of antisolvent, which governs nucleation and growth kinetics and thereby the structural and optical quality of the resulting NCs. [1] In this work, we systematically investigate how structural and chemical variations among antisolvents affect the formation of CsPbBr2 NCs. By tuning precursor compositions and antisolvent identities, we identify clear trends in crystallization behavior and photoluminescence characteristics. These experimental results are combined with a Gaussian Process regression model that encodes antisolvent geometry to predict NC emission wavelengths.[2] The model performs accurately for well-represented antisolvent classes but still faces challenges when extrapolating to sparsely sampled or previously unseen antisolvents. Our combined experimental and data-driven approach highlights the decisive role of antisolvent molecular structure in NC synthesis and demonstrates a pathway toward predictive control over perovskite nanocrystal properties.

[1]K. Frank et al., Nat. Commun. 2024, 15, 8952.
[2]N. A. Henke et al., Adv. Mater. 2025, e09472.

HL 4.3 Mon 10:15 POT/0251

Tuning Lead Halide Perovskite Nanocrystal Properties via Controllable Synthesis and Machine-Learning Insights — •Maximilian Dörfler, Leo Luber, and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Halide perovskite nanocrystals (NCs) combine high photoluminescence efficiency with tunable emission, but achieving narrow linewidths requires tightly controlled, highly monodisperse synthesis. In this work, we perform in situ observations of CsPbBr3 NC formation under ambient conditions and systematically evaluate how synthesis parameters shape their optical response. By analyzing the evolving photoluminescence spectra, we assess how reaction time, dilution, and precursor-to-antisolvent ratios jointly influence crystal growth and resultant morphology. The in situ approach allows us to track nanocrystal growth

pathways and provides the opportunity for real-time steering of the synthesis. Particular emphasis is placed on understanding the conditions under which the NCs adopt 2D versus 3D morphologies. In future work, we will employ machine-learning tools - specifically Bayesian optimization - to efficiently navigate the sparsely sampled synthesis parameter space. This data-driven strategy aims to identify regions that yield high quantum efficiencies and narrow linewidths, enabling rapid discovery of conditions that favor predominantly monodisperse nanocrystals or nanoplatelets with minimal experimental iteration.

HL 4.4 Mon 10:30 POT/0251

Scalable Perovskite-Silicon Tandem Photovoltaics by Hybrid 2-Step Inkjet Printing — •Theresa Kuechle[1], Raphael Pesch[1,2], Jinzhao Li[1,2], and Ulrich W. Paetzold[1,2] — [1]Light Technology Institute, KIT, Germany — [2]Institute of Microstructure Technology, KIT, Germany

In recent years, the power conversion efficiency (PCE) of perovskite-silicon tandem photovoltaics has improved significantly on a lab scale. For photovoltaics industry, fully scalable processes are required to ensure homogeneous thin-film formation while maintaining conformity to the bottom cell.

Here, we show a hybrid two-step process for the perovskite thin film fabrication whereby inorganic components are evaporated, followed by inkjet printing of organic components. Our approach addresses scalability challenges and highlights the suitability of inkjet printing with a green solvent for the fabrication of large textured tandem solar cells. We show that optimizing the stoichiometry is necessary and can be achieved by fine-tuning the dots per inch in the second step. Through inkjet printing parameter optimization, we achieve wide-band gap single-junction perovskite solar cells with close to 20 % PCE. Additionally, we successfully fabricate large-textured (3 to 5 μm pyramid size) tandem solar cells with an active area of 1 cm^2, achieving a single-JV-scan PCE of 27.4 %. These results underscore the potential of this hybrid fabrication process to overcome upscaling hurdles and advance the development of highly efficient tandem solar cells for industrial applications.

HL 4.5 Mon 10:45 POT/0251

A Materials Perspective on Sequential Inorganic Scaffold Deposition for Hybrid-Processed Perovskite Thin Films — •Ronja Pappenberger[1,2], Julian Petry[1,2], Alexander Welle[3,4], Tonghan Zhao[1], Alexander Diercks[2], Raphael Pesch[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 — [3]Institute of Functional Interfaces, KIT, Germany — [4]Karlsruhe Nano Micro Facility, KIT, Germany

As perovskite solar cells (PSCs) advance toward industrial-scale production, fabrication processes must combine high-throughput with simple integration. In this regard, the hybrid two-step deposition route has emerged as a promising method, allowing for conformal coatings on micron-scale textures, a critical feature for perovskite/silicon tandem photovoltaics. This work presents a fully sequential route, wherein the inorganic materials CsCl and PbI_2 are deposited separately, simplifying industrial implementation compared to co-deposition. Microstructural analysis shows that sequential deposition promotes vertical PbI_2 growth with a secondary tilted orientation, unlike the horizontal orientation from co-deposition. Elemental distribution reveals high diffusivity for Cs, formamidinium, and I, yielding a homogeneous distribution in the perovskite absorber, while Pb and Cl remain largely scaffold-bound. PSCs with a 1.69 eV bandgap achieve efficiencies of 19.3% (co-deposition) and 18.7% (sequential), highlighting fully sequential hybrid deposition as a promising route toward industrial PSC production.

15 min. break

HL 4.6 Mon 11:15 POT/0251

How stable are mixed-metal chalcohalides? — •Pascal Henkel[1], Jarno Laakso[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Xi'an Jiaotong University, Xi'an, China — [3]Technical University of Munich, Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaics,[1,2] capable of delivering high conversion efficiencies.[3] Yet, their thermodynamic stability remains largely unexplored.

We assess the thermodynamic stability of 54 MMCH compounds by modelling their phase diagrams using DFT, *pymatgen* tools from Materials Project[4] and the Alexandria Materials Database.[5] All studied MMCHs lie above the convex hull, independent of their space group ($Cmcm$, $Cmc2_1$, $P2_1/c$). Accounting for computational uncertainty (mostly from the applied exchange-correlation functional) moves a considerable fraction of MMCHs close to or below the hull. The MMCH decomposition paths follow five reactions, with $4\,M(II)_2M(III)Ch_2X_3 \leftrightarrow 2\,M(III)_2Ch_3 + 6\,M(II)X_2 + 2\,M(II)Ch$ occurring most frequently. Experiments show that compounds close to the convex hull can be synthesized, whereas compounds far from the hull decompose following the predicted reactions. Overall, our results show that MMCHs are synthesizable, but fabrication conditions need further optimisation.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Phys. Rev. Materials* **9**, 115405 (2025), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Chem. Mater.* **20**, 1798-1807 (2008). [5] https://alexandria.icams.rub.de/.

HL 4.7 Mon 11:30 POT/0251

minimizing ionic losses in DMSO-free tin-based perovskite solar cells — •Paria Forozi Sowmeeh[1], Shengnan Zuo[2], Chiara Frasca[2], Biruk Alebachew Seid[1], Sercan Ozen[1], Wentao Liu[2], Mahmoud Hussein Aldamasy[2], Yuan Zhang[3], Fengshuo Zu[2,3], Norbert Koch[2,3], Martin Stolterfoht[4], Antonio Abate[2], Artem Musiienko[2], and Felix Lang[1] — [1]Institute of Physics and Astronomy University of Potsdam, Potsdam-Golm, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Department of Physics, Humboldt University of Berlin, Berlin, Germany — [4]Electronic Engineering Department, The Chinese University of Hong Kong, Hong Kong SAR, China

The presence of mobile ions and the potential toxicity of Pb-based perovskite solar cells remain two major drawbacks for their commercialization despite their exceptional optoelectronic properties. On the other hand, Sn-based perovskites, which are believed to exhibit smaller ion-induced instabilities, have been revealed as eco-friendly perovskite counterparts, though thorough investigations are still missing. Herein, we investigate the nature of mobile ions, quantify the ionic loss within Sn-based perovskite solar cells and compare with those of Pb-based and mixed PbSn devices. We report minimal ionic losses and over 10-fold lower ion densities in DMSO-free processed Sn samples compared to Pb-based perovskites. The Sn-based devices also exhibit the lowest associated ionic losses with sustained device stability upon illumination. This study paves the way for development of innovative, stable thin film solar cells with suppressed ion migration.

HL 4.8 Mon 11:45 POT/0251

Beyond 1D: How Edge Effects Impact Ion Densities and Stability in Perovskite Solar Cells — •Jarla Thiesbrummel[1,2], Francisco Peña-Camargo[2], Bruno Ehrler[3], Dilara Abdel[4], Patricio Farrell[4], and Felix Lang[1] — [1]University of Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum zu Berlin, Berlin, Germany — [3]AMOLF, Amsterdam, Germany — [4]Weierstrass Institut, Berlin, Germany

Understanding how mobile ions redistribute within metal halide perovskites is essential for interpreting device stability and quantitative ion-density measurements. While most studies focus on ion transport along the device stack, lateral ion motion and edge effects remain relatively unexplored, despite their strong relevance, especially in small-area, lab-scale photovoltaic devices. In this work, we investigate side collection of ions at device edges and its consequences for both apparent ion densities and long-term material stability, using a combination of 2D drift-diffusion simulations and experiments.

HL 5: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

Invited Talk HL 5.1 Mon 10:30 TRE/MATH

Magnetic Order in 2D Materials Beyond Bulk Constraints — •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln

Even though exfoliated microflakes remain widely used in 2D magnetism research, their bulk origin restricts access to many potentially interesting phases, an obstacle that molecular beam epitaxy (MBE) can overcome. MBE enables the controlled synthesis of single-layer materials directly related to, yet often distinct from, their bulk counterparts.

In my talk, I will present structural characterization and discuss the mechanisms behind the formation of such novel 2D materials grown via MBE on graphene. [1-2] The emerging magnetic properties of these new 2D materials will be exemplified with two cases: Cr_2S_3-2D and Fe_2S_2-2D. Cr_2S_3 forms a covalently bonded NiAs-type structure without van der Waals gaps. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD), we show that it hosts ferromagnetic coupling within the plane with magnetic moments pointing out-of-plane, combined with A-type antiferromagnetic coupling between different Cr planes. Fe_2S_2 exhibits a unique hexagonal phase, in which Fe atoms occupy tetragonally coordinated sites. Spin-polarized STM reveals that the moments are noncollinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming a Néel state and a 2Q state.

[1] Knispel et al. Small, 2025 21, 2408044.
[2] Safeer et al. Adv. Funct. Mater. 2025, 202500907.

HL 5.2 Mon 11:00 TRE/MATH

Ab initio modeling of magnons and magnon-phonon coupling in 2D magnetic materials — Ali Esquembre-Kucukalic1[1], Khoa Le[2], Hsiao-Yi Chen[3], Ivan Maliyov[2], Jin-Jian Zhou[4], Davide Sangalli[5], and •Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Valencia, Spain — [2]CALTECH, California, USA — [3]Tohoku University, Japan — [4]Beijing Institute of Technology, Beijing, China — [5]ISM-CNR, Roma, Italy

Understanding spin-wave excitations in two-dimensional magnetic materials is essential for advancing spintronic and quantum information technologies. Chromium trihalides and related 2D magnets provide a platform where the choice of halide influences on the magnetic behavior, yet its impact on magnon properties is not completely understood. We present first-principles calculations of magnon dispersions and wave functions in monolayer Cr trihalides using the Bethe-Salpeter equation (BSE), resolving key features such as the topological gap at the Dirac point. The BSE analysis reveals that magnons originate from electronic transitions spanning a wider energy range than excitons, offering new insight magnon character and enabling the extraction of Heisenberg exchange parameters. Building on this framework, we develop an ab initio description of mag-ph coupling by deriving BSE-based mag-ph interaction matrices and applying them to monolayer CrI3 and hydrogenated graphene. We show that mag-ph and electron-phonon couplings differ markedly, identifying specific phonon modes that dominate magnon scattering.

HL 5.3 Mon 11:15 TRE/MATH

Electron-phonon interaction in transition-metal dichalcogenides — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We developed a generally applicable ab-initio implementation on top of density functional theory using a basis set of localized Gaussian orbitals. It combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation [1], which are usually neglected.

In addition to the renormalization of the electronic bands, electron-phonon interaction introduces a line broadening due to finite-lifetime effects, which have recently been incorporated into our implementation. In this presentation, we discuss our results, including those with finite-lifetime effects, for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

HL 5.4 Mon 11:30 TRE/MATH

Surface-state engineering for nonlinear charge and spin photocurrent generation — •Javier Sivianes[1], Peio Garcia-Goiricelaya[2], Daniel Hernangómez-Pérez[3], and Julen Ibañez-Azpiroz[1,4,5] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Leioa, Spain — [3]CIC nanoGUNE BRTA, San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [5]Donostia International Physics Center (DIPC), Donostia, Spain

We systematically explore the generation of nonlinear charge and spin photocurrents using spin-orbit-split surface states. This mechanism enables net DC flow along the surface plane even in centrosymmetric bulk environments like the Rashba prototype Au(111), where we characterize the main quadratic contributions by combining model predictions with density functional calculations. We further identify the Tl/Si(111) surface as a prime scenario for experimental verification; with slight doping, it develops metallic surface states featuring remarkable relativistic properties deviating from the Rashba paradigm, while the bulk remains semiconducting. Its nonlinear charge photocurrent reveals a distinct angular signature and a magnitude comparable to bulk ferroelectrics, highlighting the potential of surface-state photocurrents for low-bias optoelectronic applications. Moreover, the nontrivial spin texture of its surface states enables the generation of pure out-of-plane spin-polarized currents, offering a highly versatile nonlinear spin-filtering functionality beyond the conventional spin Hall effect.

HL 5.5 Mon 11:45 TRE/MATH

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

Spintronics offers a compelling, energy-efficient alternative to traditional electronics with potential applications in communications, sensing, and information processing. The vanadium-doped layered transition metal dichalcogenide 2*H*-WSe_2 is particularly promising as a room-temperature magnetic semiconductor with gate-tunable transport properties. Here, we use a combination of 11 eV laser, 21.2 eV He-lamp, and soft X-ray synchrotron ARPES to highlight the influence of a fairly small vanadium doping on the electronic structure of WSe_2. Both the pristine and doped compounds were grown by chemical vapor transport in our own laboratory.

HL 5.6 Mon 12:00 TRE/MATH

Engineering sulfur vacancy dimers in monolayer WS_2 — •Daniel Jansen[1], Guangyao Miao[1], Jan Keienburg[1], Jeison Fischer[1], Thomas Michely[1], Hannu-Pekka Komsa[2], and Wouter Jolie[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Sulfur vacancies [1] and sulfur vacancy dimers in nearest-neighbor distance [2] in monolayer WS_2 have been experimentally proven to yield bright and stable photon emission, thus holding promises for the development of quantum technologies.
Here we investigate dimers of sulfur vacancies in different configurations in monolayer WS_2 created with the tip of a scanning tunneling microscope [3]. Scanning tunneling spectroscopy reveals strong hybridization of the sulfur vacancy electronic in-gap states, validated by density functional theory calculations. For dimers in nearest-neighbor configuration we find that inelastically tunneling electrons can induce sulfur atom migration, resulting in a rotary motion of the dimer. This

motion is studied in detail by analyzing the emerging telegraph noise in the junction. Lastly, we elaborate on scenarios to make use of the dimer motion for the design of vacancy structures and lattices.

[1] Schuler et al., Sci. Adv. **6**, 38 (2020)
[2] Sun et al., Nature Commun. **15**, 9476 (2024)
[3] Jansen et al., Phys. Rev. B **109**, 195430 (2024)

HL 5.7 Mon 12:15 TRE/MATH

Alkali-metal doped transition metal chlorides confined in bilayer graphene: Insights from first-principles calculations — •Munawar Ali[1], Arkady V. Krasheninnikov[2], Giovanni Cantele[1], and Mahdi Ghorbani-Asl[2] — [1]Università degli Studi di Napoli "Federico II," Dipartimento di Fisica "Ettore Pancini," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The intercalation of atomic and molecular species into layered materials has emerged as a powerful strategy for synthesizing novel two-dimensional systems with tunable electronic, magnetic, and energy-storage properties. Encapsulating transition-metal halides into bilayer graphene has proven effective for stabilizing 2D magnetic phases that are otherwise thermodynamically unstable. Using density functional theory, we systematically investigate the intercalation of metal chlorides (TCl_3, T = Fe, Cu, Mo, Al) doped with alkali metals (Li, Na, K, Rb, Cs) across a range of concentrations. Li- and Na-doped $FeCl_3$, $CuCl_3$, and $MoCl_3$ monolayers exhibit the highest thermodynamic stability, whereas $AlCl_3$ remains unstable even under doping. Bader charge analyses reveal substantial charge transfer from the graphene host to the intercalated layers, particularly in the case of $CuCl_3$, which also shows the strongest binding. These findings provide a theoretical framework for understanding the stability of these heterostructures and highlight alkali-metal-intercalated graphene systems as a platform for engineering tunable 2D magnetic materials.

HL 6: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g, via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15 Location: HSZ/0003

Topical Talk HL 6.1 Mon 15:00 HSZ/0003

Charge confinement in twisted bilayer graphene — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Twisted bilayer graphene (tBLG) near the magic angle is a unique platform where the combination of topology and strong correlations gives rise to exotic electronic phases. These phases are gate-tunable and related to the presence of flat electronic bands, isolated by single-particle band gaps. This enables charge confinement and allows to explore the interplay of confinement, electron interactions, band renormalisation and the moiré superlattice, potentially revealing key paradigms of strong correlations. In this talk we will present two experiments where we study charge confinement in tBLG. First, we report on the observation of negative electronic compressibility in tBLG for Fermi energies close to insulating states. To observe this negative compressibility, we take advantage of naturally occurring twist-angle domains that emerge during the fabrication of the samples, leading to the formation of charge islands. Second, we present gate-defined single-electron transistors (SETs) in near-magic-angle tBLG with well-tunable Coulomb blockade resonances. These SETs allow to study magnetic field-induced quantum oscillations in the density of states of the source-drain reservoirs, providing insight into gate-tunable Fermi surfaces of tBLG and open the door to quantum dots and Josephson junction arrays in tBLG.

Topical Talk HL 6.2 Mon 15:30 HSZ/0003

Tuning Coulomb interactions and Hubbard bands in 1T-TaS_2 — •Anna Galler — Institute of Theoretical and Computational Physics, TU Graz, Austria — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Monolayer 1T-TaS_2 hosts a star-of-David charge-density wave (CDW) that stabilizes a low-temperature Mott-insulating state. Recent time-resolved spectroscopies indicate a coupling between the CDW amplitude mode and the electronic correlation strength, yet the role of the screened Coulomb interaction remains unclear. Using the constrained random-phase approximation, we show that the CDW amplitude modifies the bare and screened on-site interactions, leading to sizable variations in the effective Hubbard U. Our combined density-functional and dynamical mean-field theory calculations reveal that the Hubbard bands shift in concert with the CDW amplitude, and that a reduced distortion drives a transition from a Mott insulator to a correlated metal. These results demonstrate a direct link between lattice distortions and Coulomb interactions in transition-metal dichalcogenides, providing a microscopic mechanism for light-induced control of correlated phases in two-dimensional quantum materials.

Topical Talk HL 6.3 Mon 16:00 HSZ/0003

Optical signatures of interlayer electron coherence in a bilayer semiconductor — •Nadine Leisgang[1,2], Xiaoling Liu[2], Pavel Dolgirev[2], Philip Kim[2], and Mikhail Lukin[2] — [1]Phillips-Universität Marburg, Germany — [2]Harvard University, United States

Emergent strongly correlated electronic phenomena in atomically thin transition-metal dichalcogenides represent an exciting frontier in condensed matter physics, with examples ranging from bilayer superconductivity and electronic Wigner crystals to the ongoing search for exciton condensation. Here, we take a step towards the latter by reporting experimental signatures of unconventional coupling of interlayer excitons consistent with coherence between interlayer electrons in a transition-metal dichalcogenide bilayer. We investigate naturally-grown MoS_2 homobilayers integrated in a dual-gate device structure allowing independent control of the electron density and out-of-plane electric field. When the bilayer is electron-doped under conditions where tunnelling between layers is negligible, we observe that two interlayer excitons - which normally should not interact - hybridize in a way distinct from both conventional level crossing and anti-crossing. We show that these observations can be explained by quasi-static random coupling between the excitons, which increases with electron density and decreases with temperature. We argue that this phenomenon is indicative of a spatially fluctuating order parameter in the form of in-

terlayer electron coherence - a theoretically predicted many-body state that has yet to be unambiguously established experimentally outside the quantum Hall regime.

15 min. break

Topical Talk HL 6.4 Mon 16:45 HSZ/0003

Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures — •Ammon Fischer — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — Center for Computational Quantum Physics, Flatiron Institute, New York, NY 10010, USA

Moiré materials - twisted stacks of two-dimensional materials - bridge between two influential paradigms of condensed matter research: nontrivial quantum geometry and strong electron-electron interactions. In this talk, I will outline how the construction of faithful low-energy models and their successive treatment by state-of-the-art many-body techniques allows to resolve electronic order in moiré and non-moiré heterostructures from first principles. In twisted bilayers of WSe_2, functional renormalization group techniques allow to unravel the angle evolution of antiferromagnetic order and superconductivity in the crossover regime from weak-to-moderate interactions. In rhombohedral multilayer graphenes, the low-energy theory is naturally described in terms of supercell Wannier functions that span the effective $U(4) \times U(4)$ subspace of the spin, valley and layer degrees of freedom. Electronic correlations give rise to various iso-spin ordered regimes, superconductivity and charge density wave order at low electronic densities bridging to the physics of their twisted counterparts.

Topical Talk HL 6.5 Mon 17:15 HSZ/0003

Mesoscale Atomic Engineering in a Crystal Lattice — •Julian Klein — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

Controlling the arrangement of individual atoms with lasers, ion traps, and scanning probe techniques has enabled quantum simulation and computing platforms that transcend naturally occurring configurations of matter. Yet achieving comparable atomic control within a solid and at scale remains a foundational challenge, one that could revolutionize the design of artificial matter. Here, I demonstrate atomic engineering of artificial matter inside a scanning transmission electron microscope. By developing strategies to position and move the electron beam with few-picometer accuracy, deterministic control over atomic motion in both space and time is achieved. Full automation of the microscope enables the creation of three-dimensional defect superlattices in many-nanometer thick CrSBr with user-defined lattice spacing and symmetry, spanning tens of thousands of engineered sites over fields of view exceeding one hundred nanometers, all generated in under an hour. Our results establish atomic engineering in the electron microscope as a practical reality, opening unprecedented opportunities to create quantum defects and quantum phases with tunable charge and spin interactions, and to control host-lattice excitations by arranging atoms in patterns that are commensurate or incommensurate with the underlying crystal over mesoscopic, and potentially micro- or macroscopic, length scales.

HL 6.6 Mon 17:45 HSZ/0003

Interlayer electrodynamics of CDWs in van der Waals materials and heterostructures — Achyut Tiwari, Renjith Mathew Roy, Maxim Wenzel, Christian Prange, Bruno Gompf, and •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Layered transition metal dichalcogenides such as 1T-TaS_2, 2H-TaS_2 and their natural heterostructure $4H_b$-TaS_2 provide a platform for studying interlayer coupling, orbital hybridization, and charge transfer that determine collective electronic phenomena, such as unconventional superconductivity and strong electronic correlations. Temperature-dependent infrared measurements of the in-plane and out-of-plane optical response of 1T-TaS_2 across its CDW-driven metal-insulator transition are combined with DFT calculations. We find that a quasi-1D instability that induces interlayer dimerization is responsible for the MI-transition. Furthermore, spectroscopic ellipsometry combined with an anisotropic Bruggeman effective medium approximation reveals that metallic domains evolve in a strongly anisotropic way and often extend along the out-of-plane direction as the transition proceeds.

When 1T-TaS_2 is stacked between 1H-TaS_2, forming a natural heterostructure of $4H_b$-TaS_2, charge transfer occurs between the layers, that can be tuned with temperature, and which is related to the CDW in 1T-TaS_2 layer. We conclude that the phase transition in 1T-TaS_2 is inherently three dimensional, despite its layered structure, and that interlayer coupling is essential for its electronic structure and phase behavior both individually and in heterostructures.

HL 6.7 Mon 18:00 HSZ/0003

Enhancing Plasmonic Superconductivity in Layered Materials via Dynamical Coulomb Engineering — •Yann in 't Veld[1], Mikhail I. Katsnelson[2,3], Andrew J. Millis[4,5], and Malte Rösner[2,6] — [1]I. Institute of Theoretical Physics, Universität Hamburg, Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [3]Constructor Knowledge Institute, Constructor University, Bremen, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, United States of America — [5]Department of Physics, Columbia University, New York, United States of America — [6]Faculty of Physics, Bielefeld University, Bielefeld, Germany

Conventional Coulomb engineering, through controlled manipulation of the environment, offers an effective route to tune the correlation properties of atomically thin van der Waals materials via static screening. Here we present tunable *dynamical* screening as a method for precisely tailoring bosonic modes to optimize many-body properties. We show that "bosonic engineering" of plasmon modes can be used to enhance plasmon-induced superconducting critical temperatures of layered superconductors in metallic environments by up to an order of magnitude, due to the formation of interlayer hybridized plasmon modes with enhanced superconducting pairing strength. We determine optimal properties of the screening environment to maximize critical temperatures. We show how bosonic engineering can aid the search for experimental verification of plasmon mediated superconductivity.

HL 7: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

HL 7.1 Mon 15:00 HSZ/0204

A virtual super-moiré: $MnBr_2$ on graphene on Ir(110) — Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], •Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

$MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of $Gr/MnBr_2/Ir(110)$ is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice – two lattices not in contact with each other. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110), and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110). Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2/Gr/Ir(110)$ super-moiré.

HL 7.2 Mon 15:15 HSZ/0204

Magnetism of monolayers of $FeCl_2$ and $FeBr_2$ Epitaxially Grown on Bi_2Se_3 — •Sebastien E. Hadjadj[1], Weibin Li[2], Pierluigi Gargiani[2], Cinthia Piamonteze[3], Oleksandr Stetsovych[4], Pavel Jelínek[4], Maxim Ilyn[1], and Celia Rogero[1] — [1]Materials Physics Center(MPC - CFM), Donostia, Spain — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Two-dimensional transition metal dihalides exhibit novel magnetic and electronic properties. By combining 2D magnetic semiconductors with topological insulators (TIs) novel quantum and spintronic phenomena can be investigated. Here, we report the uniform and epitaxial growth of monolayer $FeCl_2$ and $FeBr_2$ on the TI Bi_2Se_3. Structural and electronic characterization via LEED, STM, and STS measurements revealed a material-specific moiré pattern resulting from lattice mismatch, as well as a position-independent bandgap of 4 eV. Synchrotron-radiation-based XAS and XMCD measurements confirm robust ferromagnetic order down to the monolayer limit, with an intrinsic reduction of the effective spin magnetic moment by 40-50%. These magnetic vdW heterostructures provide a platform for investigating magnetic proximity effects and moiré-induced modifications of topological surface states. [1] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847*9856,(2023) [2] S. Kerschbaumer et al., Adv. Science, e08262,(2025)

HL 7.3 Mon 15:30 HSZ/0204

Rise and fall of 1T-TaS_2: Epitaxial growth of monolayer TaS_2 on Au(111) — •Lars Buss[1], Cathy Sulaiman[1], Raquel Sánchez-Barquilla[1], Iulia Cojocariu[2], Marcin Szpytma[3], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy — [3]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland — [4]Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional TaS_2 has attracted extensive research interest due to its ability to exhibit electron correlation effects, including charge density waves (CDWs). In particular, 1T-TaS_2 is of interest as it shows a CDW at room temperature. However, when grown on metal substrates, only 2H-TaS_2 has been reported. To elucidate the reasons for the apparent lack of 1T-TaS_2 growth in the literature, we have investigated the growth of TaS_2 on Au(111) employing *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED) as well as X-ray photoemission electron microscopy (XPEEM) [1]. We show that at elevated temperatures TaS_2 nucleates and grows in the metastable 1T-TaS_2 phase, which transforms into the stable 2H-TaS_2 phase via a temperature-activated process and then continues to grow at a considerably lower rate. Furthermore, we observe CDW-like ordering in 1T-TaS_2/Au(111), though it is suppressed in 2H-TaS_2/Au(111).

[1] L. Buß et al. Phys. Rev. Materials **9**, 074006 (2025).

HL 7.4 Mon 15:45 HSZ/0204

Band-Like Transport and its Modulation by Nitrogen Doping in Transferable Semi-Conducting 2D-imine Covalent Organic Framework — •Vijay Bahadur Yadav, Diksha Srivastava, Satya Veer Singh, Itu Pandey, Manabendra Chandra, and Thiruvancheril G. Gopakumar — Indian Institute of Technology Kanpur

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are promising semiconductors for thin-film electronics and sensing due to their extended in-plane π-conjugation, enabling efficient charge transport. Here, we investigate two highly crystalline 2D imine COF films synthesised via quasi-equilibrium Schiff base condensation. By selecting molecular precursors, we tuned the nitrogen content, producing COFs with ten and six nitrogen atoms per unit cell (10N-COF and 6N-COF). The films are chemically stable in organic solvents and water, mechanically robust, and transferable onto various substrates, allowing fabrication over areas of tens of square centimeters. Electrical measurements using silver electrode arrays show linear current*voltage behaviour, indicating band-like transport, with consistent responses across multiple regions. The conductivity of 10N-COF is ~36 times higher than that of 6N-COF. Density functional theory calculations reveal similar band gaps but enhanced band dispersion near the Fermi level in 10N-COF, improving charge carrier mobility. Nitrogen incorporation thus effectively tunes charge transport in 2D COFs.

HL 7.5 Mon 16:00 HSZ/0204

Co_2S_2: a new 2D material and its phase transitions — •Abdallah Karaka, Max Wolfertz, Affan Safeer, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra high vacuum conditions, 2D materials can be synthesized under conditions far from equilibrium for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: $P\bar{3}m1$ trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing with a lattice constant of 3.66 ± 0.05 Å and a height of 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.52 ± 0.05 Å and a height of 11.7 Å. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase.

HL 7.6 Mon 16:15 HSZ/0204

Tailored growth of 2D alloy transition metal dichalcogenides with tunable optical and electrical properties using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Nhat Lam Duong[1], Julian Picker[1], Rahul Sharma[1], Christof Neumann[1], Mona Sedighi[2], Johannes Biskupek[2], Muhammad Sufyan Ramzan[1], Caterina Cocchi[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Doping or alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) provides a promising route to tune the optical, magnetic, and electronic properties. Here, we present a liquid-precursor-based chemical vapor deposition (CVD) for the controlled growth of large-area monolayer $(V_xW_zMo_{1-x-y})S_2$ alloys with tunable optical and electrical properties. Comprehensive characterization using atomic force microscopy, transmission electron microscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy, and ab initio calculations confirms the structural and optical quality. Notably, PL shows a noticeable defect exciton peak at room temperature in the V-doped monolayer. Furthermore, by adjusting the composition, we modulate the carrier type of these monolayers from n-type to p-type or even make the monolayers metallic for high vanadium concentrations, which is deduced from electrical transport measurements and density

functional theory calculations. This work demonstrates high potential of liquid-precursor CVD as a platform for the tailored growth of complex 2D TMD alloys for next-generation optoelectronic devices.

HL 7.7 Mon 16:30 HSZ/0204

CVD growth and characterization of WSe_2 monolayers on Au(111) and their conversion to Janus SeWS — •Julian Picker[1], Jonas Brandhoff[2], Maximilian Schaal[2], Felix Otto[2], Christof Neumann[1], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) exhibit distinctive optical and electronic properties in the two-dimensional monolayer limit. Recently, Janus TMDs have attracted significant attention because their asymmetric chalcogen composition breaks the out-of-plane symmetry and enables properties not attainable in conventional TMDs. In this work, we initially investigate the structural and electronic characteristics of WSe_2 monolayers grown on Au(111) via ambient-pressure chemical vapor deposition (CVD). Surface-sensitive techniques - including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and angle-resolved photoelectron spectroscopy (ARPES) - were employed to characterize the properties of these monolayers. Subsequently, the WSe_2 monolayers were transformed into Janus SeWS monolayers through selective chalcogen replacement at the WSe_2/Au interface. A comparative analysis reveals the structural and electronic differences between the two systems.

HL 7.8 Mon 16:45 HSZ/0204

Controlling polymorphism in the growth of 2D manganese sulfide on graphene via substrate interaction — •Max Wolfertz, Abdallah Karaka, Nicolas Georgopoulos, Oktay Güleryüz, Affan Safeer, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide on graphene/Ir substrates grown via molecular beam epitaxy. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and - spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: manganese sulfide in trigonal CuI-structure (space group P-3m1) and MnS in thin platelets of a cubic rock-salt structure (space group Fm-3m). Their in-plane lattice parameters are 4.16 Å, and 3.63 Å respectively. We show that the substrate exerts a strong influence on the phase selected. While the growth on Gr/Ir(111) results in a large share of cubic MnS, the Gr/Ir(110) substrate favors the formation of single layer trigonal manganese sulfide. Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

HL 7.9 Mon 17:00 HSZ/0204

Low Temperature MOCVD Growth of two-dimensional InSe and InSe/WS2 Heterostructures — •Robin Guenkel, Nils Langlotz, Matvei Kislitsyn, Juergen Belz, and Kerstin Volz — mar.quest|Marburg Center for Quantum Materials and Sustainable Technologies, Philipps University Marburg, Germany

Two-dimensional van der Waals heterostructures offer powerful opportunities for engineered optoelectronic functionality, particularly when type-II band alignment enables efficient charge separation and interlayer transitions. InSe and WS* are especially promising in this regard because their band structures allow for the formation of a type-II interface at the Γ point, which avoids momentum mismatch. This is an essential requirement for robust radiative processes in 2D stacks. This talk presents a low-temperature metal-organic chemical vapor deposition (MOCVD) approach for synthesizing high-quality InSe and vertically integrated InSe/WS2 heterostructures. Using DTBSe and TMIn at 350 °C, we synthesize homogeneous, single-phase InSe films on 2-inch sapphire substrates and extend the process to directly grow on monolayer WS2. Atomic force microscopy, Raman spectroscopy, and energy-dispersive X-ray spectroscopy provide insight into the morphology, crystallinity, and composition of the films, offering a detailed understanding of the growth behavior and the influence of the substrate surface chemistry.

HL 7.10 Mon 17:15 HSZ/0204

Synthesis of Vertically Stacked 2D-hBN/Borophene Heterostructures on Ir(111) via Intrinsic Segregation — •Marko Kriegel, Karim Omambac, Smruti Mohanty, Birk Finke, Frank-J. Meyer zu Heringdorf, and Michael Horn-von Hoegen — University Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Lotharstr. 1, 47057 Duisburg, Germany

Research efforts on 2D materials increasingly target complex architectures built from high-quality heterostructures. A key challenge remains the reliable and scalable in-situ fabrication of such systems. In this work, we use high-resolution spot-profile analysis LEED (SPA-LEED) and -microscopy (LEEM) to investigate a synthesis route for an hBN/borophene heterostructure on Ir(111) based on *intrinsic segregation*. At elevated temperatures, boron dissolves into the Ir subsurface region during exposure to the borazine precursor $B_3N_3H_6$ in a CVD process [1], thereby creating a boron reservoir. Increasing the precursor pressure drives the chemical balance toward formation of a complete hBN layer across the Ir surface [2]. Upon cooldown, the decreasing boron solubility induces segregation, resulting in the growth of a continuous borophene layer beneath the hBN overlayer. This one-step CVD approach establishes a promising, scalable pathway for the controlled synthesis of high-quality 2D heterostructures. [1] K. Omambac et al., ACS Nano **15** (2021) 7421 [2] K. Omambac et al., ACS Nano **17** (2023) 17946

HL 7.11 Mon 17:30 HSZ/0204

MBE growth and characterization of high-quality monolayer MoS2 on stepped Au surface — •Sayan Debnath, Ram Prakash Pandeya, Konstantin Shchukin, Patrik Staudenmayer, and Alexander Grüneis — Optoelektronische Materialien Institut für Festkörperelektronik, TU Wien, 1040 Wien, Austria

In the present work, we investigate the growth of sub-monolayer MoS2 on Au(788) and Au(111), using molecular beam epitaxy. Sample growth quality is characterized using low-energy electron diffraction, X-ray photoemission spectroscopy, and scanning electron microscopy. Furthermore, a comparative study of the electronic properties was performed by studying the band structure using angle-resolved photoemission spectroscopy (ARPES), and the vibrational properties were measured by angle-resolved polarized Raman (ARPR) spectroscopy.

Our study reveals superior crystalline quality, with fewer S deficiencies, and better azimuthal order of MoS2 grown on the stepped Au(788) substrate compared to the Au(111). In the case of ARPES, we observed more resolved band dispersion on MoS2/Au (788), confirmed by probing the spin-orbit splitting at the Brillouin zone boundary (K point). On the other hand, ARPR of the first Raman mode E2g on MoS2/Au (788) deviates from the symmetry of freestanding MoS2, suggesting the effect of the stepped surface on the vibrational properties. We discuss the role of increased catalytic activity at step edges in promoting the growth of high-quality TMDCs, such as MoS2 and WS2, on stepped surfaces.

HL 8: Ultra-fast Phenomena I

Time: Monday 15:00–18:15 Location: POT/0006

HL 8.1 Mon 15:00 POT/0006

Lightwave Engineering of Excitonic States in an Atomically Thin Semiconductor — •Omer Kneller[1], Niloufar Nilforoushan[1], Matthias Knorr[1], Markus Borsch[2], Fabian Mooshammer[1], Mackillo Kira[2], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan 48109, USA

Coherently shaping excitonic states holds great potential for novel optoelectronics and quantum information processing. Yet, their femtosecond-scale coherence time substantially constrains coherent control. Here, intense phase-stable carrier waves of light resonantly drive the excitonic 1s-2p states in monolayer $MoSe_2$ faster than their natural decoherence rate, driving the excitonic system into multiple Rabi oscillations that occur during a single cycle of light. The dynamics are probed by injecting excitons into the 1s state using femtosecond NIR pulses and measuring the induced high-order sideband emission. The signal exhibits surprising spectro-temporal signatures that are reproduced by many-body simulations and a reduced two-level model, exposing the dominant role of the 1s-2p sub-system, even under these extreme driving conditions. An intuitive Floquet analysis links these features to light-induced avoided crossings between higher-order Floquet replicas of the driven two-level system. Our results bridge lightwave electronics in quantum materials, attosecond science, and atomic physics, and establish an exciting new route to shaping many-body quantum correlations at optical clock rates.

HL 8.2 Mon 15:15 POT/0006

Light-Induced Polarization Switching in R-Stacked Bilayer WSe_2 — •Xiangzhou Zhu, Stefono Mocatti, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Sliding ferroelectricity in two-dimensional van der Waals materials enables polarization control by relative layer motion, offering a promising platform for novel memory devices. Recent works show that strong laser pulses can reverse the polarization of such systems by driving shear phonons, but the required interlayer sliding and structural distortions limit the achievable switching speed. Here, we demonstrate a purely electronic pathway for light-induced polarization reversal in rhombohedrally stacked bilayer transition-metal dichalcogenides (TMDs). With constrained density-functional theory (cDFT), we find that photoexcited carrier densities below 0.2 e per unit cell are sufficient to switch the intrinsic ferroelectric dipole without interlayer sliding in WSe_2. This occurs because photoexcitation induces an imbalanced charge redistribution between the layers, which generates a counter-dipole. Using real-time semiconductor Bloch equation simulations, we shows that the total polarization can reverse by light within a few hundred femtoseconds. Furthermore, time-dependent charge analysis reveals that this ultrafast switching is primarily driven by a localized dipole rearrangement around the tungsten sites. These results establish a new mechanism for electronic control in 2D ferroelectrics, relevant for high-speed volatile memory applications.

Funded by the European Union (ERC, DELIGHT, 101052708)

HL 8.3 Mon 15:30 POT/0006

Ultrafast excitonic coherent oscillations in monolayer tungsten disulphide — •Jorge Cervantes Villanueva[1], Davide Sangalli[2], Alberto García-Cristóbal[1], and Alejandro Molina-Sánchez[1] — [1]Institut de Ciència dels Materials (ICMUV), Universitat de València, Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain — [2]Istituto di Struttura della Materia-CNR (ISM-CNR), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy

Understanding coherent excitonic dynamics in two-dimensional semiconductors is crucial for advancing quantum-optical technologies. Monolayer transition metal dichalcogenides (TMDs) provide an ideal platform due to their strong Coulomb interactions and large exciton binding energies. We perform ab initio pump-probe simulations by propagating the time-dependent density matrix under the influence of overlapping pump and probe fields, capturing the generation and detection of coherent excitons on femtosecond timescales. Focusing on monolayer WS2 with a pump tuned between the A and B excitons, we observe ultrafast oscillations arising from coherent coupling among multiple excitonic states, including the intermediate A* resonance. Exploiting the balance between exciton populations, we propose a scheme to control the coherent response, realizing an optical switch with potential applications in quantum information. These results establish ab initio pump-probe modeling as a predictive tool for characterizing and manipulating coherent excitonic states.

HL 8.4 Mon 15:45 POT/0006

Carrier-envelope phase control of ultrafast photocurrents in layered MoS2 — •Johannes Schmuck[1,2], Björn Sinz[1,2], Nina Pettinger[1,2], Sergey Zherebtsov[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Munich Center of Quantum Science and Technology, Munich, Germany

We demonstrate carrier-envelope-phase (CEP)-controlled photocurrents in mono-, bi-, and tri-layer MoS2 driven by few-cycle laser pulses. The photocurrent in the two-terminal devices scale quadratically with the field amplitude, indicating perturbative carrier dynamics in the weak-field regime distinct from strong-field tunnelling [1]. Our results extend light-field-sensitive current control from bulk dielectrics, semiconductors, and graphene to two-dimensional transition-metal dichalcogenides, highlighting their potential for electric-field sensitive optoelectronics.

[1] J. Schmuck et al., submitted, arXiv preprint arXiv:2511.08148 (2025).

HL 8.5 Mon 16:00 POT/0006

Development of an ultrafast scanning electron microscope — •Leon Kross[1], Benjamin Schröder[1], Niklas Wemheuer[1], Leon Brauns[1], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Ultrafast electron microscopy (UEM) enables the study of structural and electronic dynamics in solid-state materials with nanoscale spatial and femtosecond temporal resolution [1]. While UEM at high ($>$ 30 keV) and low ($<$ 1keV) electron energies is well established, ultrafast experiments in the intermediate energy regime have been less employed thus far, despite their potential to bridge the gap between surface- and bulk-sensitive measurements. Here, we present a new ultrafast scanning electron microscope (USEM), designed to investigate physical phenomena in the energy range from 1 to 30 keV. The modular architecture supports diverse experimental configurations and detection schemes, spanning from standard SEM operation modes - such as secondary- and backscattered-electron imaging - to more advanced techniques including cathodoluminescence or electron diffraction. In this contribution, we show example measurements, highlighting the performance of our USEM and its potential for exploring ultrafast physical phenomena. [1] A. Feist et al. Ultramicroscopy, 176, 63-73 (2017)

HL 8.6 Mon 16:15 POT/0006

Ultrafast X-ray diffraction shows dynamics of phase domains make V2O3 films remember photoexcitation ten thousand times longer — •Oleg Gorobtsov[1,2], Yoav Kalcheim[3,4], Ziming Shao[1], Anatoly Shabalin[3], Nelson Hua[3], Daniel Weinstock[1], Ryan Bouck[1], Mathew Seaberg[5], Diling Zhu[5], Oleg Shpyrko[3], Ivan Schuller[3], and Andrej Singer[1] — [1]Cornell University, USA — [2]University of Tübingen, Germany — [3]University of California San Diego, USA — [4]Technion-Israel Institute of Technology, Israel — [5]SLAC National Accelerator Laboratory, USA

Metal-insulator transitions in vanadium oxides combine electronic and structural phase transformations. Memory effects present during the phase transition in thin V2O3 films make the material a candidate for neuromorphic computing, but what role does the structural phase heterogeneity play in memory? We used an X-ray free-electron laser probe to show that strain feedback on structural phase domain nucleation increases the metal-insulator relaxation time after an optically induced insulator-metal transition from nanoseconds to a hundred microseconds. The dynamic range and precision of the experiment distinguish that the memory follows a stretched exponential law, not a power law. We also provide an experimental basis for the transition incubation

times during the first 10 picoseconds after the excitation.

15 min. break

HL 8.7 Mon 16:45 POT/0006

Carrier-envelope phase modulation of ultrafast photocurrents in indium nitride — •Maximilian A. Gruber, Alexandra V. Nemmaier, Johannes Schmuck, Abhilash Ulhe, Gregor Koblmüller, and Alexander W. Holleitner — Walter Schottky Institute and Physics Department, Technical University of Munich, Munich, Germany

Few-cycle laser pulses allow for electronic transport at petahertz frequencies, where the carrier-envelope phase (CEP) controls the direction and strength of the ultrafast photocurrents. While such effects have been studied in graphene, bulk semiconductors and wide-bandgap dielectrics, their realization in group-III nitrides remains largely unexplored. We demonstrate CEPdependent photocurrents in InN devices excited by stabilized 6 fs optical pulses. The response reveals fieldsensitive contributions and strong interface effects close to the contacts of the investigated sample, highlighting the microscopic role of builtin electric fields in device architecture. The results position InN as a promising platform for CEP-controlled ultrafast transport.

HL 8.8 Mon 17:00 POT/0006

Towards studying quasi-particle interactions on the nanoscale — •Philipp Kessler, Matthias Hensen, Victor Lisinetskii, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Investigating the properties and dynamics of quasi-particles is essential for tailoring material functionality in device fabrication. Nonlinear optical spectroscopy has become a standard tool for probing ultrafast single quasi-particle dynamics. However, the use of high light intensities, intended to improve the signal-to-noise ratio, can also generate multiple quasi-particle excitations, which may interact with each other. As a result, the measured signal consists of overlapping contributions from single- and multi-particle processes, each with distinct dynamics. To address this, our group recently developed the intensity cycling technique, which enables the experimental separation of individual perturbative orders in nonlinear light–matter interaction [1,2]. Here, we report our progress in extending this technique to time-resolved photoemission electron microscopy (PEEM) to study quasi-particle interactions with high spatial resolution. In our PEEM setup [3], we employ a 680 nm pump pulse with variable intensity for excitation and a 340 nm probe pulse for photoemission. This scheme allows us to investigate organic thin films of molecular aggregates, focusing primarily on exciton–exciton annihilation as a probe of exciton diffusion.

[1] P. Malý et al., Nature 616, 280-287 (2023).
[2] J. J. Krich et al., J. Phys. Chem. Lett. 16, 5897-5905 (2025).
[3] B. Huber et al., Rev. Sci. Instrum. 90, 113103 (2019).

HL 8.9 Mon 17:15 POT/0006

Watching polarons form in real time — •Victor Garcia-Herrero and Fabio Caruso — Institute of Theoretical Physics and Astrophysics, Christian-Albrechts University of Kiel, Germany

Polaron formation in pump-probe experiments is a fast, non-equilibrium process arising from the coupled motion of electrons and lattice vibrations, leading to the emergence of a localized quasiparticle. A new first-principles quantum-kinetic approach is introduced to track the real-time dynamics of electrons and the lattice under electron-phonon interactions. We applied this method to the polar insulators MgO and LiF, and determine the characteristic timescales of polaron localization and identify its unique dynamical signatures. The results reveal distinct dynamical signatures of polaron formation and establish clear, practical criteria for its detection in ultrafast pump-probe experiments, providing a direct connection between theory and experiment.

Founded by Marie Skłodowska-Curie Actions (MSCA), TIMES network.

HL 8.10 Mon 17:30 POT/0006

Dynamic control of electron correlations in photodoped charge-transfer insulators — •Thomas C. Rossi[1,2], Nicolas Tancogne-Dejean[3], Malte Oppermann[1,4], Michael Porer[5], Arnaud Magrez[6], Rajesh V. Chopdekar[7], Yayoi Takamura[7], Urs Staub[5], Renske M. van der Veen[2], Angel Rubio[3,8], and Majed Chergui[1,9] — [1]LSU and LACUS, EPFL, Lausanne, Switzerland — [2]PS-ADLU, HZB, Berlin, Germany — [3]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [4]Department of Chemistry, University of Basel, Switzerland — [5]SLS, PSI, Villigen, Switzerland. — [6]Crystal Growth Facility, EPFL, Lausanne, Switzerland — [7]Department of Materials and Science Engineering, UC Davis, USA — [8]ICC and CCQ, Simons Foundation Flatiron Institute, New York, USA — [9]Elettra-Sincrotrone, Trieste, Italy

Tuning the electronic properties of materials is typically achieved by altering their chemical composition or thermodynamic parameters. An alternative route relies on ultrafast light excitation, which can create transient phases such as light-induced superconductivity and hidden insulator-to-metal transitions. In this talk, I will present evidence of light-driven dynamic screening of electron correlations in a prototypical charge-transfer insulator, nickel oxide (NiO). The excited state, characterized by weakened electron correlations, is metastable for hundreds of picoseconds. The high degree of control achieved over both the energetic and temporal aspects of electronic correlations offers a promising path toward full optical control of the electronic properties of correlated systems and the Mott transition.

HL 8.11 Mon 17:45 POT/0006

Photostriction-Driven Phase Transition in Layered Chiral $NbOX_2$ Crystals: Electrical-Field-Controlled Enantiomer Selectivity — •Jorge Cardenas-Gamboa[1], Martin Gutierrez-Amigo[2], Aritz Leonardo[3], Gregory A. Fiete[4], Juan L. Mañes[3], Jeroen van den Brink[1], Claudia Felser[5], and Maia G. Vergniory[3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden — [2]Department of Applied Physics, Aalto University — [3]Donostia International Physics Center — [4]Northeastern University, Boston — [5]Max Planck Institute for Chemical Physics of Solids

Controlling the handedness of crystal structures is essential for developing next-generation optical, electronic, and information technologies. Yet, achieving reversible and selective control over crystal chirality remains a major challenge. In this work, we demonstrate a two-step pathway for enantiomer selectivity in layered chiral $NbOX_2$ (X = Cl, Br, I) crystals based on photostriction-driven phase transitions. *Ab-initio* simulations reveal that optical excitation is capable of inducing a structural phase transition in $NbOX_2$ from the monoclinic ($C2$) ground state to the higher-symmetry ($C2/m$) structure. In the resulting transient high-symmetry state, an applied electric field breaks the residual inversion-symmetry degeneracy, selectively stabilizing one enantiomeric final state configuration over the other. Our results establish a combined optical-electrical control scheme for chiral materials, enabling reversible and non-contact enantiomer selection with potential applications in ultrafast switching, optoelectronics, and chiral information storage.

HL 8.12 Mon 18:00 POT/0006

Efficient Two-Dimensional Spectroscopy Simulations including Realistic Pulse Shapes, Overlapping, and Time-Ordering Effects — Rémi Gilliot[1,2], •Matteo Russo[1], Alexander Blech[1], Manuel Joffre[2], Christiane Koch[1], and Hélène Seiler[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Institut Polytechnique de Paris, Palaiseau, France

We present an approach capable of simulating Two-Dimensional Electronic Spectroscopy (2DES) spectra with arbitrary pulse shapes, pulse overlap, and pulse ordering on a standard laptop. Under the assumption of simple dephasing, we show that the 2DES emitted signal - a convolution integral that involves pulses* fields and material response and that is traditionally challenging to evaluate numerically - reduces to a simple product of three independent one-dimensional integrals. This fortunate simplification makes this approach fast and computationally less expensive than others, while still capturing most of the realistic pulse-dependent effects listed above. Finally, we benchmark the effectiveness of this approach on three canonical systems - an anharmonic oscillator, two coupled oscillators, and a dimer model - studying how spectral phase distortions and strongly non-Gaussian pulse shapes, such as those produced by hollow-core fibers, can influence the 2DES emitted signal.

HL 9: Oxide Semiconductors: Growth and Fabrication

Time: Monday 15:00–16:30 Location: POT/0051

HL 9.1 Mon 15:00 POT/0051

Growth of rutile GeO_2 by plasma-assisted suboxide molecular beam epitaxy — Alexander Karg[1], •Satjawoot Phiwondee[1], Manuel Alonso-Orts[1,2], Marco Schowalter[1], Andreas Rosenauer[1,2], Martin Eickhoff[1,2], and Patrick Vogt[3] — [1]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

The interest in ultra-wide bandgap (UWBG) semiconductors for high-power electronic applications is rapidly increasing, for which rutile germanium dioxide (r-GeO_2) is a promising material. It possesses excellent properties: a bandgap of 4.6 eV [1], thermal conductivity of 51 W/mK [1], and a breakdown electric field of 7 MV/cm [1] and theoretical bipolar dopability [2].
This work reports on the growth of r-GeO_2 on m-plane Al_2O_3 substrates using plasma-assisted suboxide molecular beam epitaxy, using a SnO_2 buffer, followed by a r-$Ge_xSn_{(1-x)}O_2$ buffer to stabilize the r-GeO_2 phase. The growth of r-GeO_2 on those buffer layers is demonstrated and the responsible nucleation mechanism is investigated in detail. Characterization was performed by atomic force microscopy (AFM) and high resolution X-ray diffraction (HRXRD). Selected r-GeO_2 layers were analyzed by scanning transmission electron microscopy (STEM).
[1]: M. Labed et al., Materials Today 83, 513-537 (2025)
[2]: S. Chae et al., Appl. Phys. Lett. 114, 102104 (2019)

HL 9.2 Mon 15:15 POT/0051

Wafer-scale transfer and integration of tungsten-doped vanadium dioxide films — •Guanyi Li[1,2], He Ma[2], and Peter J. Klar[1] — [1]University of Giessen Institute of Physic, Giessen, 35392, Germany — [2]Beijing University of Technology, Institute of Information Photonics Technology, Beijing 100124, People's Republic of China

The trend in modern optoelectronic devices is towards greater flexibility, wearability, and multifunctionality. This demands more flexible fabrication methods of functional layers. Vanadium dioxide (VO_2), with its metal-insulator transition (MIT) at 68 °C, is of interest for many optoelectronic devices. However, high-quality VO_2 usually needs to be grown at T >450 °C in an oxygen-containing atmosphere implying a low compatibility with many optoelectronic device concepts, e.g., on flexible substrates. Here, we use a layer-by-layer transfer method of wafer-scale tungsten-doped VO_2 films, which enables sequential integration of VO_2 films with different MIT temperatures (down to 40 °C) onto arbitrary substrates. By stacking multiple VO_2 films with different doping levels of W, a quasi-gradient-doped VO_2 architecture can be achieved, effectively broadening the MIT temperature window and reducing the hysteresis of VO_2. Such integrated VO_2 films find a wide scope of applications, e.g., flexible temperature indicator strips, infrared camouflage devices, nonreciprocal ultrafast light modulators, or smart photo actuators. Our work promotes the development of more flexible and tunable optoelectronic devices integrated with VO_2.

HL 9.3 Mon 15:30 POT/0051

Growth and characterization of ultra-wide bandgap oxide semiconductor $LiGa_5O_8$ — •Nazar Masiuta, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Lithium gallium oxide ($LiGa_5O_8$) has been recently grown as an ultra-wide bandgap oxide semiconductor with robust p-type conductivity using mist chemical vapor deposition[1]. This discovery suggests application of the material in high-power electronics by forming p-n junctions with n-type α-Ga_2O_3, β-Ga_2O_3, and isostructural γ-Ga_2O_3. However, establishing the origin of p-type conductivity of lithium gallium oxide remains an experimental challenge[2], while a theoretical prediction argues that neither native nor dopant defects in $LiGa_5O_8$ could be responsible for it[3]. We analyze the influence of pulsed laser deposition growth parameters on the quality of lithium gallium oxide films on different substrates. The structural, optical, and electrical characterization of $LiGa_5O_8$ is performed to determine the type of conductivity and its origin in the fabricated samples.
[1] K. Zhang *et al.*, Adv. Electron. Mater. **11**, 2300550 (2025).
[2] K. Zhang *et al.*, APL Mater. **13**(4), 041104 (2025).
[3] J. L. Lyons, J. Appl. Phys. **135**(16), 165705 (2024).

HL 9.4 Mon 15:45 POT/0051

(N:)CuBi2O4 photocathode thin films for photoelectrochemical water splitting — •Miriam J. Fehrenbach[1,2], Dominic Rapf[1,2], Katarina S. Flashar[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Photoelectrochemical (PEC) water splitting is a promising pathway to carbon-neutral solar fuels. While metal oxides are well explored as photoanodes, complementary photocathodes remain scarce. Potential candidates are Cu-based oxides, which naturally exhibit p-type conductivity. Among them, copper bismuthate (CuBi*O*) is a promising material [1], combining a visible-light bandgap with high photocurrent onset potentials [2], but suffering from poor charge transport [1]. To address this limitation, we developed a reactive co-sputtering and annealing process to synthesize high-quality, nitrogen-modified CuBi*O* thin films. We systematically examine structural and optical effects of nitrogen incorporation and find a significant improvement in PEC activity. To understand this enhanced performance, we investigate the charge carrier transport properties with (photo)conductivity measurements. [1] J. K. Cooper et al., Chem. Mater., 2021, 33, 3, 934*945. [2] N. T. Hahn et al., J. Phys. Chem. C, 2012, 116, 10, 6459*6466.

HL 9.5 Mon 16:00 POT/0051

High-throughput combinatorial synthesis of perovskite-type materials for solar applications — •Clemens Petersen, Andreas Rosnes, and Holger von Wenckstern — Centre for Materials Science and Nanotechnology, University of Oslo, Norwa

Recently, combinatorial deposition methods have increasingly gained attention due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. Our combinatorial pulsed laser deposition (c-PLD) approach enables the fabrication of material libraries on a single substrate, spanning wide compositional spaces with precise spatial control. Combined with high-throughput characterization techniques (HTC) such as spatially resolved UV-VIS spectroscopy and X-ray diffraction, the properties of complex materials can be rapidly mapped with high chemical resolution and minimal effort. We demonstrate the potential of c-PLD for accelerating the discovery of perovskite oxides for solar-energy-related applications. Using the $SrTiO_3$*$BaTiO_3$ (STO-BTO) system as an example, we showcase rapid screening of structural and optical properties on small area spatially addressable material libraries (SAML) covering the full composition range. In addition, STO-BTO SAMLs enable systematic strain engineering of functional perovskite materials. The tunable band structures and suitability for catalytic processes such as photoelectrolysis and proton-coupled electron transfer render titanate perovskites promising candidates for solar fuel production. Our results underline the capability of c-PLD and HTC workflows to efficiently identify and optimize oxide perovskites for sustainable energy technologies.

HL 9.6 Mon 16:15 POT/0051

Pulsed laser deposition of rutile GeO_2 thin films — •Hannah Dichelle, Sofie Vogt, Marius Grundmann, and Holger von Wenckstern — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Rutile germanium-oxide has recently come into focus as an ultrawide bandgap material which is predicted to offer the possibility of ambipolar doping. [1,2] The stabilization of rutile phase GeO_2 is challenging due to the similar formation energies of the amorphous phase and α-Quarz phase.[2] We present GeO_2 thin films fabricated by pulsed laser deposition at heater temperatures >450°C. To facilitate the crystallization in the rutile phase (Sn, Ge)O_2 buffer layers are grown on sapphire and TiO_2 substrates at heater temperatures >600°C. Both ternary $Sn_xGe_{1-x}O_2$ buffer layers and vertically composition graded buffer layers are used to stabilize the rutile phase. The structural properties of rutile phase GeO2 thin films are investigated as a function of the growth temperature and oxygen pressure.

[1] Chae *et al.*, Appl. Phys. Lett. 114, 102104 (2019)

[2] Shimazoe *et al.*, Jpn. J. Appl. Phys. 64, 050903 (2025)

HL 10: 2D Materials II – Electronic and transport properties (joint session HL/TT)

Time: Monday 15:00–16:30 Location: POT/0081

HL 10.1 Mon 15:00 POT/0081

Ballistic electrostatic graphene superlattices using He ion-milled etching masks — •Rebecca Hoffmann[1], Giulia Piccinini[1], Julien Barrier[1], David Barcons Ruiz[1], Hanan Herzig Sheinfux[1], Takashi Taniguchi[2], Kenji Watanabe[3], Adrian Bachtold[1,4], and Frank H.L. Koppens[1,4] — [1]ICFO-Institut de Ciencies Fotoniques, Castelldefels, Spain. — [2]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

An electrostatic superlattice is created by applying a periodic electrostatic potential to a material using patterned gates or dielectrics, leading to tunable band structure reconstruction. This approach enables free design of the superlattice geometry and lattice period. While high mobility has been observed, signatures of ballistic transport (e.g. negative resistance in cross geometry, transverse magnetic focusing) remain to be reported. Here, we present a nanofabrication technique combining Helium ion milling of etching masks with damage-free etching of graphite gates [1]. Using these gates in a graphene heterostructure creates an electrostatic superlattice which preserves graphene's high mobility. We report superlattice features. The high electronic quality is confirmed by transverse magnetic focusing and device-size limited mean free path.

[1]D. Barcons Ruiz, et al., Nat. Commun. 13, 6926 (2022)

HL 10.2 Mon 15:15 POT/0081

Tomographic flow regime in the 2D Corbino disk geometry — •Grigorii Starkov — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

2D materials offer a unique test ground to study electron transport regimes dominated by the electron-electron collisions. This makes them the perfect platform to observe the electron hydrodynamic flows.

Not so long ago, it has been realized that precisely in 2D, the electron collisions constrained due to Pauli blocking result in the appearance of the long lived collective modes with odd angular character. The corresponding novel transport regime has been dubbed "tomographic".

In the recent experiment [2], magnetoresistance in Corbino-shaped graphene devices was used to disentangle different contributions to the electron transport and to determine viscosity. The obtained temperature-dependence thereof has been linked to the tomographic flow. However, the analysis is based on the bulk expressions for the conductivity and does not treat boundary corrections in detail. At the same time, boundary layers have been shown to be anomalously large in the tomographic flow regime [3].

To take into account the boundary effects, I analyze the magnetoresistance in the 2D Corbino disk geometry across different regimes, using the linearized Boltzmann equation.

[1] P. Ledwith et al, Phys. Rev. Lett. 123, 116601 (2019) [2] Y. Zeng et al, arXiv:2407.05026 (2025) [3] N. Ben-Schachar, J. Hoffmann, arXiv:2503.14431 (2025)

HL 10.3 Mon 15:30 POT/0081

Pulsed-gate spectroscopy of the electron-hole block- ade in bilayer graphene double quantum dots — •Lars Mester[1,2], Hubert Dulisch[1,2], Katrin Hecker[1,2], Konstantinos Kontogeorgiou[3], Samuel Möller[1,2], Leon Stecher[1], Kenji Watanabe[4], Takashi Taniguchi[5], Fabian Hassler[3], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [3]JARA- Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [4]Research Center for Functional Materials, Na- tional Institute for Materials Science, Namiki, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Namiki, Japan

Pauli blockade is an established read-out mechanism for quantum-dot (QD) spin qubits. Using bilayer graphene (BLG) as a platform offers advantages such as a tunable valley degree of freedom. Recently, a strong spin-valley blockade was demonstrated in an electron-hole BLG double quantum dot (DQD) using time-averaged transport measurements. Here, we employ pulsed-gate spectroscopy by pulsing between the (0e, 0h) and (1e, 1h) charge configurations. Comparison with simulations allows us to identify unconventional higher-order tunneling as the dominant blockade-lifting mechanism, with timescales governed by QD-lead coupling and the number of accessible states. Our results provide direct access to blockade-lifting dynamics in a BLG DQD, offering relavant insights for the development of future BLG-based qubits.

HL 10.4 Mon 15:45 POT/0081

Temperature Dependent Electrical Transport in Thin $SnSe_2$ — •Lars Thole[1], Aarti Lakhara[2], Preeti A. Bhobe[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Indore, Simrol, 453552, India

The two-dimensional material $SnSe_2$ shows special temperature dependent behavior [1], which has not been understood to its full capacity as of now.

We fabricated thin samples of $SnSe_2$ and investigated its electrical transport behavior in regards to its temperature dependence [2]. These samples show a metal-insulator transition with a metallic state for higher temperatures. The low-temperature transport regime is dominated by variable-range hopping. Additionally, the influence of defect states in these samples is investigated by looking at the thickness dependence for different samples [3].

[1] C. Guo, et al., Appl. Phys. Lett. 109, 203104 (2016).
[2] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. arXiv: 2507.14536 (2025).
[3] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. Phys. Rev. B 112, 235401 (2025).

HL 10.5 Mon 16:00 POT/0081

Polarization resolved Electron Spin Resonance in two-dimensional electron systems — •Daniiar Khudaiberdiev[1], Alexey Shuvaev[1], Michail Glazov[2], Anton Shchepetilnikov[3], Viacheslav Muravev[3], Christian Reichl[4], Werner Wegscheider[4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Technische Universität Wien, 1040 Vienna, Austria — [2]St. Petersburg, Russia — [3]Chernogolovka, Russia — [4]Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland

Electron spin resonance (ESR) has long served as a powerful probe of g-factor anisotropy, spin-orbit interactions, hyperfine coupling, and collective many-body spin phenomena in two-dimensional electron systems (2DESs). Most prior studies detect ESR in the photoresistance of Hall bars, where the excitation-field distribution and polarization are distorted, complicating the analysis of the excitation conditions.

In contrast, we report polarization-resolved ESR in sub-THz transmission using a quasi-optical setup and large-area samples that ensure high polarization purity. First we study the 2DES hosted in a 4.5-nm AlAs quantum well with a single isotropic valley. The selection rules indicate that Dresselhaus spin-orbit coupling mediates the electric-dipole-active spin absorption. Further we examine systems with more complex spectra such as wide AlAs wells with an active pseudospin, HgTe and InAs quantum wells with low effective mass and strong spin-orbit coupling enhancing the effects.

HL 10.6 Mon 16:15 POT/0081

First-Principles Investigation of Electronic Transport in 2D GaSe: Backward Diodes, p-i-n FETs, and Double-Gate MOSFETs — •Dogukan Hazar Ozbey and Engin Durgun — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey

In this study, we present a comprehensive first-principles investigation of charge transport in monolayer GaSe nanodevices by combining density functional theory with the nonequilibrium Green's function (DFT + NEGF) formalism. Three representative architectures, namely p–n junctions, p–i–n field-effect transistors (FETs), and double-gate MOSFETs, are systematically analyzed. Our calculations reveal that GaSe p–n junctions display an unconventional backward diode response, in which reverse currents within the ± 1 V window exceed forward currents owing to tunneling-assisted transport, as evidenced by the projected local density of states. When configured as p–i–n FETs, electrostatic gating allows selective control over tun-

neling conduction. Moderate gate biases suppress the reverse current, whereas stronger gating reactivates and amplifies it. Finally, double-gate GaSe MOSFETs with channel lengths of approximately 5 nm exhibit competitive figures of merit that meet or surpass the ITRS-2028 high-performance benchmarks, achieving an on/off ratio of 1.2×10^4, intrinsic delay time of 0.24 ps, and power–delay product of only 0.06 fJ·μm^{-1}. Our results highlight GaSe as a single 2D semiconductor capable of integrating backward-diode behavior with high-speed transistor operation.

HL 11: Focus Session: Quantum Emitters in 3D Semiconductors

Quantum emitters in 3D semiconductors play a crucial role in many applications. In this focus session, we focus on the latest developments for their use in quantum technologies. In addition to the well-known NV center in diamond, there are a number of other defect centers in various semiconductor systems that hold great potential for quantum sensing, quantum cryptography, and/or quantum information technology. Today's research focuses on the discovery of new centers, their properties, synthesis, and their microscopic origin. For the latter, ab initio methods are often used, and the material systems span silicon, nitrides, carbides, and other semiconductors with large band gaps.

Organized by Carsten Ronning and Jan Meijer

Time: Monday 15:00–18:15 Location: POT/0251

Invited Talk HL 11.1 Mon 15:00 POT/0251
Quantum Repeater Hardware made from Silicon Carbide — •Jörg Wrachtrup — Center for Applied Quantum Technologies, University of Stuttgart

Distributing entanglement via quantum repeaters is a formidable challenge. Memory-based approaches require quantum emitters that couple strongly to optical fields, and at the same time demand stationary qubits with excellent coherence properties. Colour centres in solids meet these requirements remarkably well and are therefore leading contenders in the field. However, existing solutions are either technically demanding or result in limited network efficiency.

Silicon carbide (SiC) offers several advantages over current approaches. Most notably, SiC is a wafer-scale material with excellent nanophotonic properties and hosts defects with outstanding spin coherence. In this talk, I will highlight recent progress in incorporating colour centres into nanophotonic structures and achieving efficient photon extraction. In addition, the electron spins of these colour centres can be coupled to nuclear spin qubits with exceptional coherence properties. I will discuss this coupling and its use as quantum memories for repeaters.

Invited Talk HL 11.2 Mon 15:30 POT/0251
Diamond based quantum sensing for drug testing — •Romana Schirhagl — University Medical Center Groningen, Groningen, the Netherlands

Free radical generation plays a key role in the mechanisms of action of many different drugs. Additionally, free radical generation offers a powerful biomarker to quantify the drug efficacy. However, free radicals are difficult to measure since they are short lived and reactive. Diamond based quantum sensing offers a possible solution to this problem. We have demonstrated recently that we can predict which drugs might work in clinical samples. Here we can either measure stress responses [1] (as for instance caused by anti-cancer drugs or anti-biotics) or reduction of oxidative stress [2] (as caused by anti-inflammatory drugs, certain inhibitors or anti-oxidants). We tested synovial fluid from rheumatoid arthritis and osteoarthritis patients. We can clearly differentiate the two groups which differ in their responsiveness to Piroxicam. Such ex-vivo measurements can be used for diagnostic purposes, to predict the effectiveness of a drug or to elucidate its mechanism of action. In my talk I will show different examples of how quantum sensing can be used in drug development. 1 Tian, Y., Nusantara, A.C., Hamoh, T., Mzyk, A., Tian, X., Perona Martinez, F., Li, R., Permentier, H.P. and Schirhagl, R., 2022. ACS Applied Materials & Interfaces, 14(34), pp.39265-39273. 2 Sigaeva, A., Shirzad, H., Martinez, F.P., Nusantara, A.C., Mougios, N., Chipaux, M. and Schirhagl, R., 2022. Small, 18(44), p.2105750.

Invited Talk HL 11.3 Mon 16:00 POT/0251
The oxygen-related ST1 centre in diamond: a room temperature coherently controllable electron spin — •Sebastien Pezzagna — Applied Quantum Systems, Universität Leipzig, Leipzig, Germany

The development of quantum information and technologies has rapidly evolved from the beginning of the century. Nowadays, there exists a variety of defects and host crystals which are suitable for applications in quantum computing, sensing or communication, such as the nitrogen-vacancy (NV) centre in diamond. However, the reliable and scalable employment of such a system requires the ability to produce it on demand together with a deep understanding of its optical and spin properties, as well as charge states and close by environment.

In this presentation, we will discuss the so-called ST1 centre in diamond, one of the few defect centres possessing a coherently controllable electron spin at room temperature. We will first show how we could identify the nature of the ST1 centre and how it can then be produced on demand. We will then emphasize the large spin readout contrast and charge state stability which characterise the ST1 centre, and how this compares to the well-known NV centre. Finally, we will highlight the peculiarities of the ST1 centre, supported by optical spectroscopy and by investigations of the hyperfine interactions with surrounding carbon-13 nuclear spins and with the oxygen-17 nuclear spin within the centre itself.

15 min. break

Invited Talk HL 11.4 Mon 16:45 POT/0251
Silicon quantum emitters emitting in the optical telecommunication range for scalable quantum photonic circuits — •Yonder Berencén — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Silicon has recently emerged as a promising host for single-photon emitters operating at telecom wavelengths, offering a pathway toward scalable quantum photonic technologies on a CMOS-compatible platform. In this invited talk, I will provide an overview of the most relevant intrinsic and extrinsic-based quantum emitters in silicon, including the W, G, T, and C centers as well as erbium. I will discuss their optical and spin properties, deterministic creation via broad-beam ion implantation and focused ion beam implantation, and recent progress toward realizing spin-optical interfaces in the optical telecom bands. Particular emphasis will be placed on single-emitter spectroscopy, demonstration of optically detected magnetic resonance (ODMR) in silicon at telecom wavelengths, and the integration opportunities enabled by silicon*s mature photonic and electronic fabrication ecosystem. Finally, I will outline a roadmap toward fully monolithic silicon quantum photonic integrated circuits that combine single emitters with on-chip photonic routing and a groundbreaking approach for silicon-based single-photon detectors at the telecom range.

Invited Talk HL 11.5 Mon 17:15 POT/0251
Advances in materials processing for quantum sensing — •Adam Gali — HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — Budapest University of Technology and Economics, Budapest, Hungary

For more than a decade, our first-principles studies have suggested that neutral divacancy defects in silicon carbide (SiC) could provide such an alternative. These defects can be excited in the infrared and

emit in the second biological window, making them intrinsically attractive for biological sensing. The next step is to engineer the SiC surface and introduce shallow divacancy species suitable for nanoscale sensing. Under ambient conditions, however, SiC readily oxidizes and forms a high density of optical and paramagnetic defects at the interface, necessitating new materials-processing strategies. We have shown with first-principles calculations that the ODMR contrast of divacancy centers can be enhanced through strain engineering, a prediction verified experimentally by our collaborators. Additionally, we proposed replacing the native oxide with carbon-chain terminations to prevent oxidation. Our simulations revealed that such surfaces serve as ideal hosts for shallow divacancy quantum sensors capable of detecting external paramagnetic species [1]. This theoretical proposal has since been experimentally demonstrated by our collaborators, paving the way toward non-invasive, room-temperature quantum sensor devices.

[1] Non-invasive bioinert room-temperature quantum sensor from silicon carbide qubits, Pei Li et al., Nature Materials, 24, 1913 (2025).

HL 11.6 Mon 17:45 POT/0251

Generation of Vacancy-Based Colour Centres in 4H-Silicon Carbide for Quantum Nanophotonics with Optically Active Spins — •Leonard K.S. Zimmermann[1,2], Jonah Heiler[1,2], Samuel C. Eserin[3], Matthias Rupp[1], Ella B. Schneider[3], Jean-Nicolas Audinot[1], Steven K. Clowes[3], Ben N. Murdin[3], Stephan Kucera[1], and Florian Kaiser[1,2] — [1]Luxembourg Institute of Science and Technology (LIST), Esch-sur-Alzette, Luxembourg — [2]University of Luxembourg, Esch-sur-Alzette, Luxembourg — [3]Advanced Technology Institute, University of Surrey, United Kingdom

Silicon carbide (SiC) has emerged as a promising colour centre platform for scalable quantum systems based on nanophotonics and -electronics. Integration into nanophotonic circuits requires sub-micron three-dimensional positioning control of colour centres, achievable via ion implantation to create vacancies followed by thermal annealing. Spin-optical quantum coherence properties vary significantly with implantation parameters. We present initial results from an ongoing implantation-annealing study for generating VSi and VSiVC colour centres in 4H-SiC. Helium and Neon are implanted with varied doses at different energies, and different annealing processes for colour centre formation are investigated. We summarise single-emitter yield and show basic spin coherence measurements for the different processes. Our study highlights parameters necessary for optimal generation conditions of colour centres in 4H-SiC.

HL 11.7 Mon 18:00 POT/0251

Controlled generation of color centers in MBE-grown AlN for quantum photonics applications — •Meysam Saeedi[1], Duc V. Dinh[1], Andrey N. Anisimov[2], Mingyun Yuan[1], Georgy V. Astakhov[2], and Alberto Hernández-Mínguez[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

The large electronic band gap of aluminium nitride (AlN), its compatibility with CMOS technology, and the presence of defect centers acting as quantum light sources in the visible spectral range, make this material attractive for applications in integrated quantum photonics. In this contribution, we demonstrate the controlled generation of optically active defect centers in AlN thin films grown on 4H-SiC by molecular beam epitaxy (MBE). To this end, we compare the photoluminescence (PL) spectra of pristine AlN samples grown under both N-rich and Al-rich conditions with their corresponding PL spectra after H-ion irradiation and annealing. We show that achieving high-purity single-photon emitters in samples grown under N-rich conditions is hindered by a broad background PL, primarily arising from native oxygen-related defect complexes already present in as-grown samples. However, the PL background is reduced by more than one order of magnitude by turning the MBE growth conditions from N-rich to Al-rich regimes. These results outline a clear pathway toward the engineering of integrated, high-purity quantum emitters in epitaxial AlN.

HL 12: Heterostructures, Interfaces and Surfaces: Photonics

Time: Monday 16:45–18:30 Location: POT/0051

HL 12.1 Mon 16:45 POT/0051

Surface patterning for high index contrast AlOx/GaAs distributed Bragg reflectors — •Frederike Jaeschke[1,2], Yurii Kutovyi[1,2], Nils von den Driesch[1,2], Serhii Darahan[3], Christoph Krause[1], Benjamin Bennemann[1], Frank Vewinger[3], and Alexander Pawlis[1,2] — [1]Peter Gruenberg Institute, Forschungszentrum Juelich GmbH, Juelich, Germany — [2]JARA-Fundamentals of Future Information Technology, Juelich-Aachen Research Alliance, Aachen, Germany — [3]Institut für Angewandte Physik, Universitaet Bonn, Bonn, Germany

Enhancing the refractive index contrast between the constituent materials in a distributed Bragg reflector (DBR) leads to stopband broadening and an increase in the attainable reflectivity for a given number of layer pairs, thereby mitigating the impact of growth-induced thickness variations on optical properties. One promising approach involves the post-growth wet-oxidation of AlAs to amorphous AlOx, which substantially increases the index contrast relative to conventional AlAs/GaAs stacks. In this talk, we present optimization of the AlAs/GaAs DBR growth parameters alongside different substrate patterning approaches which facilitate controlled lateral oxidation for micrometer-scale AlOx/GaAs pillar structures. We compare the optical properties of wet-oxidized AlOx/GaAs and as-grown AlAs/GaAs DBRs to explore the potentials and limitations of such pre-structuring concepts for realizing high index contrast DBRs with decreased growth times and improved layer thickness accuracy.

HL 12.2 Mon 17:00 POT/0051

Improving Photoelectrochemical Nitrate Reduction on Copper (I) Oxide Electrodes — •Maximilian Christis[1,2], Jasmin Zitzmann[1,2], Saswati Santra[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The photoelectrochemical (PEC) nitrate reduction reaction (NO_3RR) offers a green approach for simultaneous production of ammonia (NH_3) and removal of the wastewater pollutant nitrate (NO_3*) in ambient conditions. Copper (I) oxide (Cu_2O) was recently reported to be active for both electrochemical (EC) and PEC NO_3RR, but its practical application is limited by stability issues. Thus, optimal reaction conditions that balance NH_3 selectivity and catalyst stability remain to be established. In the current investigation, we find that alkaline electrolytes enhance Cu_2O-catalyzed PEC NO_3RR compared to neutral conditions, and higher NH_3 selectivity is achieved at lower applied potentials. However, under illumination and at potentials < 0.3 V vs. RHE, the catalyst rapidly reduces to metallic Cu, favoring EC rather than PEC NO_3RR. To address this challenge, we are exploring possible strategies to reduce in-situ decomposition of Cu_2O photocathodes, aiming to enable their long-term use for solar NH_3 synthesis.

HL 12.3 Mon 17:15 POT/0051

InGaN/GaN nanowire arrays for photoelectrochemical biosensors — •Hannah Nell, Genrietta Steingelb, Rudolfo Hötzel, Ruben Neelissen, Stephan Figge, Tim Grieb, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them promising candidates for use as electrochemical biosensors [1]. In this work, we analyse the simultaneous detection by photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, enabling sensitive and selective sensing of redox-active biomolecules. However, the performance of the NW photoelectrode is constrained by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly driven by non-passivated surface states. The deposition of ultra-thin metal oxide films is a possibility to suppress such effects. The influence of TiO2 as a surface coating on the sensor properties was analysed by photoelectrochemical characterisation, demonstrating how surface modifications can affect the sensor performance in biochemical envi-

ronments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003)

HL 12.4 Mon 17:30 POT/0051

Metal-oxide passivation for high-efficiency photoelectrochemical devices — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Thin metal-oxide protection layers are crucial in highly efficient III-V photoelectrochemical (PEC) devices to suppress interfacial recombination and ensure long-term stability. Here, we study TiO_2 layers deposited on AlInP/GaInP(100) photoabsorbers, examining how surface preparation prior to atomic layer deposition and the Ti-precursor chemistry affect the chemical composition and band alignment at the TiO_2/III-V heterointerface, as well as the TiO_2 bulk and surface properties. Before TiO_2 deposition, the native oxide on AlInP(100) was removed by wet-chemical etching. TiO_2 films were grown using either TTIP or $TiCl_4$ with H_2O at various substrate temperatures. X-ray photoelectron spectroscopy was used to characterize the interface and TiO_2 bulk composition. We observe precursor-dependent differences in contaminant species in the TiO_2 bulk, at the surface, and at the TiO_2/III-V heterointerface, while their concentration is strongly influenced by deposition temperature and post-growth annealing. Finally, we correlate precursor choice and initial surface condition with TiO_2 layer stability in aqueous electrolytes under PEC-relevant conditions.

HL 12.5 Mon 17:45 POT/0051

Lab-Based NAP-XPS for Probing Photoelectrochemical Interfaces: The Case of $CuBi_2O_4$ — •Katarina S. Flashar[1,2], Miriam Fehrenbach[1,2], Gaurav Anand[3], Dominic Rapf[1,2], Barbara A. J. Lechner[3], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Chemistry Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Understanding complex (photo)electrochemical conversion processes at functional interfaces requires in situ and operando characterization. A tool enabling such investigations is near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). In this contribution, we discuss the implementation of an open liquid cell for (photo)electrochemical measurements at our recently installed, lab-based NAP-XPS system (SPECS). As a photoelectrochemical case study, we examine sputter-deposited copper bismuthate ($CuBi_2O_4$) thin film photocathodes in contact with water-based electrolytes. We thereby extend previous NAP-XPS studies on light- and gas-dependent changes in surface chemistry of $CuBi_2O_4$ [1] to the solid|liquid interface under illumination. These investigations demonstrate the capability of our lab-based NAP-XPS to probe functional interfaces of energy materials under working conditions, offering an accessible and flexible alternative to synchrotron-based measurements. [1] F. E. Oropeza et al., ACS Appl. Energy Mater. 2019, 2, 6866 - 6874.

HL 12.6 Mon 18:00 POT/0051

Correlative Atomic Force Microscopy to Understanding Local Charge Transport in Photoanodes — •Sven Doll and Johanna Eichhorn — Technical University of Munich, Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.
To this end, we correlate Kelvin probe force microscopy (KPFM) and (photo)conductive atomic force microscopy (AFM) to study the local band bending, charge accumulation, as well as variations in the generated surface photovoltage and (photo)conductivity. However, analyzing nanostructured materials with complex morphologies is not trivial, because effects such as topographic crosstalk can significantly influence the results obtained. To overcome these issues, we leverage 2^{nd} eigenmode and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventional tapping mode KPFM techniques. For $BiVO_4$, one of the most extensively studied metal oxide photoanode materials, we compare different KPFM modes and correlate the results with local conductivity measurements to gain insights into local semiconductor properties at grain boundaries or different crystal facets. Overall, the gained nanoscale insights will put forward the development of rational design strategies to enhance the macroscale durability and efficiency of solar energy conversion systems.

HL 12.7 Mon 18:15 POT/0051

Persistent UV-Induced Work Function Control at Atomic Layer Deposited TiO_2 /Ta_2O_5 Bilayer Interfaces — •Julius Kühne[1,2], Tim Rieth[1,2], Katarina S. Flashar[1,2], Johannes Dittloff[1,2], Lukas Wolz[2], Johanna Eichhorn[2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching

While atomic layer deposition (ALD) enables precise fabrication of ultrathin metal-oxide films, the mechanisms governing charge-carrier dynamics and band alignment at their interfaces often remain poorly understood. Oxide bilayers grown by ALD offer a versatile platform to characterize and tune defects that dictate interface energetics and charge transfer. Here, we examine the optical tuning of interface energetics in ultrathin ALD TiO_2/Ta_2O_5 bilayer films. A persistent -0.4 eV work-function (WF) shift is observed via contact potential difference (CPD) measurements after 275 nm illumination, with polarity reversal upon bilayer sequence inversion. This response arises from long-lived deep-trap filling, suggesting oxygen-vacancy migration. Capacitance-voltage (C-V) profiling, in-plane transport, and Kelvin probe force microscopy (KPFM) confirm vertical and lateral charge redistribution, while X-ray photoelectron spectroscopy (XPS) probe defect states. The results indicate that WF modulation originates from charge trapping by deep-trap states at the interface, offering insight into defect-driven effects in oxide heterointerfaces.

HL 13: 2D Materials III – Interlayer excitons

Time: Monday 16:45–18:30 Location: POT/0081

HL 13.1 Mon 16:45 POT/0081

Robust Interlayer Exciton Interplay in twisted Van der Waals Heterobilayer and Heterotrilayer on a Broadband Bragg Reflector up to Room Temperature — •Bhabani Sankar Sahoo, Shachi Machchhar, Avijit Barua, Martin Podhorsky, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The MoSe2/WSe2/WSe2 Heterotrilayer (HTL) shows higher interlayer exciton (IX) emission intensity compared to the MoSe2/WSe2 heterobilayer (HBL) due to the additional WSe2 monolayer in the HTL, which improves interlayer coupling and provides additional radiative pathways. However, its coupling strength and thermal stability with increasing temperature remain unexplored. Here, we fabricate HTL and HBL using H-type stacking with twist angle of 55 and 50 for the MoSe2/WSe2 and WSe2/WSe2 heterostructures (HS) on the chirped distributed Bragg reflectors (cDBRs) centered at 800 nm. Photoluminescence (PL) emission at 4K shows that HTL exhibits more than 10-fold higher intensity compared to HBL. The temperature-dependent valley polarization reveals the interplay of triplet and singlet IX in the PL emission of the HBL and Indicates the influence of band modulation on the PL emission of the HTL. The temperature-dependent lifetime further provides insights into the different decay processes in both the HS, highlights the variations in optical performance between HTL and HBL HS with temperature. Additionally, through the combined effect of controlled stacking angles and the use of cDBR substrate, we successfully achieve room temperature IX across both regions of HS.

HL 13.2 Mon 17:00 POT/0081

Ring-shaped Interlayer Exciton Ensembles in $MoSe_2/WSe_2$ Heterostructures by Laguerre-Gaussian Excitation — •Mirco Troue[1], Johannes Figueiredo[1], Gabriel Mittermair[1], Jonas Kiemle[1], Hendrik Lambers[2], Ana Senkić[2], Ursula Wurstbauer[2], and Alexander Holleitner[1] — [1]Walter Schottky Institute and Physics Department, TU Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Institute of Physics, Münster University, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Transition metal dichalcogenide monolayers exhibit strong light-matter interactions, which promotes them as ideal candidates for novel 2D optoelectronic applications. A vertical stacking into van der Waals heterostacks leads to the formation of long-lived interlayer excitons in adjacent layers. We report on ring-shaped ensembles of interlayer excitons in $MoSe_2/WSe_2$ heterostructures as excited by an optical Laguerre-Gaussian mode. The excitation is achieved with the help of a spatial light modulator. A hyperspectral analysis of the exciton photoluminescence suggests that the excitation scheme generates a non-uniform momentum distribution that favors the accumulation of high-energy excitons in the rings' center. We discuss the mechanisms leading to such a distribution, including exciton-exciton interaction, phase-space filling, and incomplete thermalization.

HL 13.3 Mon 17:15 POT/0081

Exciton-Exciton Interactions in Van der Waals Heterobilayers — •Tommy Schulz[1], Alexander Steinhoff[2], and Frank Jahnke[1] — [1]University of Bremen, Bremen, Germany — [2]Carl von Ossietzky University Oldenburg, Oldenburg, Germany

Optically excited van der Waals heterobilayers hosting long-lived interlayer excitons provide a compelling platform for exploring correlated electronic states. In this work, we compute the exciton energy shift as a function of excitation density and temperature. This shift arises from a subtle interplay of various many-body interaction processes, each of which contributes either a blue- or a redshift, corresponding to repulsive or attractive interactions, respectively. By incorporating the fermionic substructure of excitons as well as dynamical screening effects, we show that the commonly assumed dominant repulsive dipole-dipole interaction is almost perfectly compensated. This finding challenges the simple picture of a purely bosonic exciton gas. Moreover, we identify a crossover from attractive to repulsive behavior at elevated exciton densities. Comparing these results - obtained using first-principle band structures and Coulomb matrix elements - with those from a simpler two-band model highlights the importance of a material-realistic description of the electronic states.

HL 13.4 Mon 17:30 POT/0081

Optical Injection and Detection of Long-Lived Interlayer Excitons in van der Waals Heterostructures — •Anna Seiler, Alperen Tügen, Arthur Christianen, Martin Kroner, and Atac Imamoglu — ETH Zurich, Switzerland

Interlayer excitons, electron-hole pairs spatially separated between two layers of 2D materials, have gained attention for their potential to enable the exploration of bosonic quantum phases. A promising strategy to stabilize these excitons is to use transition metal dichalcogenide (TMD) bilayer structures, where the two TMD layers are separated by a few layers of hexagonal boron nitride (hBN), effectively isolating itinerant electrons and holes. While these systems have primarily been studied through transport measurements, challenges such as difficulties in making ohmic contacts to TMD monolayers and the lack of photoluminescence have limited their broader exploration. Here, we demonstrate optical generation of dipolar interlayer excitons in TMD bilayers separated by up to seven hBN layers. We observe that the 2s excitons in the individual layers remain intact in the presence of opposite charges in both layers, suggesting that the oppositely charged carriers are strongly bound, forming stable interlayer excitons. We measure exciton lifetimes up to ten microseconds, underscoring their potential for studying exotic quantum phases such as Bose-Fermi mixtures and excitonic condensates [1]. These phenomena can be accessed through optical spectroscopy, enabling future exploration.

[1] A. Tüğen, A. M. Seiler, et al., Phys. Rev. Lett. DOI: https://doi.org/10.1103/stgs-2s58

HL 13.5 Mon 17:45 POT/0081

Influence of hBN spacer layers on atomic reconstruction in $MoSe_2/WSe_2$ heterostructures probed by electron microscopy — •Johannes Figueiredo[1,2], Kaiyuan Chen[3], Aubrey Penn[4], Mirco Troue[1,2], Sebastian Loy[1,2], Frances M. Ross[3], Julian Klein[3], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]MCQST — [3]Massachusetts Institute of Technology — [4]MIT.nano

Atomically thin hexagonal boron nitride (hBN) tunnelling barriers in transition metal dichalcogenide (TMD) heterobilayers have recently facilitated the observation of macroscopic interlayer exciton phases interpreted as possible condensation and superfluid phenomena. However, such hBN spacer layers are also expected to modify moiré-driven atomic reconstruction. Here, we resolve local stacking configurations, lattice relaxation patterns and twist-angle variations across encapsulated $MoSe_2/WSe_2$ heterobilayers using a combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF STEM), convergent-beam electron diffraction and four-dimensional STEM. Our analysis shows that the presence and thickness of the hBN spacer layers alter the balance between elastic relaxation and interlayer registry, producing a reconstruction landscape that differs qualitatively from that of directly contacted $MoSe_2/WSe_2$ bilayers. We also discuss how the resulting changes in structural homogeneity tune the moiré potential experienced by interlayer excitons and outline the implications for realizing spatially uniform macroscopic exciton phases in TMD-based quantum devices.

HL 13.6 Mon 18:00 POT/0081

Spin-bright interlayer exciton and trion ground state in Janus transition metal dichalcogenide bilayers from first-principles — •Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], Marta Prada[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

We investigate bilayer Janus transition metal dichalcogenides using ab initio many-body screened configuration interaction calculations [1] and find that MoSSe–WSSe and WSSe–WSSe, with Se–S interfaces, exhibit spin-allowed interlayer exciton and trion ground states [2], in contrast to the spin-forbidden ground states of conventional transition metal dichalcogenides bilayers. This distinctive behavior is driven by the intrinsic structural asymmetry and interface-induced polarization, which significantly modify the electronic band structure. Moreover, we demonstrate that external mechanical strain allows to tune the optical properties of these excitons, enabling precise control over their

brightness and potential applications in optoelectronic devices.

[1] Mørch Nielsen, C.E., Fischer, F. & Bester, G. *npj 2D Mater. Appl.* **9**, 11 (2025)
[2] Mørch Nielsen, C.E., Fischer, F., Prada, M. & Bester, G. *2D Mater.* **12** 045015 (2025)

HL 13.7 Mon 18:15 POT/0081

Interplay of excitonic species in vertical and lateral transition metal dichalcogenide heterostructures — •Sai Shradha[1], Md. Tarik Hossain[2], Nicole Engel[1], Luc Oswald[1], Julian Führer[1], Daria Markina[1], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Lessingstr. 10, D-07743 Jena, Germany

The properties of transition metal dichalcogenides (TMDs) can be extended beyond those offered by individual monolayers by combining different monolayers to create heterostructures. Vertically stacked heterostructures host quasi-particles such as interlayer and Moiré excitons. In lateral heterostructures (LHs), where monolayers of different materials are covalently bonded in the plane of their atoms, unidirectional exciton transport and the formation of charge-transfer excitons can be realized [1]. Chemical vapour deposition (CVD) has been a key fabrication technique for LHs. This work investigates composite CVD-grown $MoSe_2$-WSe_2 heterostructures consisting of both lateral and vertical interfaces, providing a single platform to study exciton dynamics across different interface types. Optical spectroscopy reveals efficient interlayer coupling in such structures, resulting in a uniquely strong interlayer exciton emission. Several spectroscopy techniques, including magneto-optics, are employed to characterize and shed light on exciton dynamics in such systems.

[1] S. Shradha et. al., arXiv, 2510.21422 (2025)

HL 14: Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)

Time: Tuesday 9:30–10:45 Location: HSZ/0105

Invited Talk HL 14.1 Tue 9:30 HSZ/0105

Simulating high-temperature superconductivity in a triangular moiré lattice — •Kin Fai Mak — Luruper Chaussee 149 Bldg. 900 (MPSD), 22761 Hamburg, Germany

Moiré materials built on transition metal dichalcogenide semiconductors have emerged as a tunable platform for simulating the Hubbard model on a triangular lattice. A natural question arises: Can the platform be tuned to yield a phase diagram similar to that in high-temperature cuprate superconductors? In this talk, I will discuss the emergence of high-temperature superconductivity near the Mott transition in a triangular moiré lattice with intermediate coupling strength. The emergent doping-temperature phase diagram looks remarkably similar to that in cuprate superconductors. I will also discuss the evolution of the phase diagram by tuning the band structure of the material by gating. The results could provide a new angle for understanding the phenomenon of high-temperature superconductivity in strongly correlated materials.

HL 14.2 Tue 10:00 HSZ/0105

Engineering Hubbard models with gated two-dimensional moiré systems — •Yiqi Yang[1], Yubo Yang[2], Miguel Morales[3], and Shiwei Zhang[3] — [1]Lund University, Lund, Sweden — [2]Hofstra University, New York, USA — [3]Flatiron Institute, New York, USA

Lattice models are powerful tools for studying strongly correlated quantum many-body systems, but their general lack of exact solutions motivates efforts to simulate them in tunable platforms. Recently, a promising new candidate has emerged for such platforms from two-dimensional materials. A subset of moiré systems can be effectively described as a two-dimensional electron gas (2D EG) subject to a moiré potential, with electron-electron interactions screened by nearby metallic gates. In this talk, we present the realization of lattice models in such systems [1]. We show that, by controlling the gate separation, a 2D EG in a square moiré potential can be systematically tuned into a system whose ground state exhibits orders analogous to those of the square lattice Hubbard model, including the stripe phase. Furthermore, we study how variations in gate separation and moiré potential depth affect the ground-state orders. A number of antiferromagnetic phases, as well as a ferromagnetic phase and a paramagnetic phase, are identified.We then apply our quantitative downfolding approach to triangular moiré systems closer to current experimental conditions, compare them with the square lattice parameters studied, and outline routes for experimental realization of the phases.

[1] arXiv:2508.13314

HL 14.3 Tue 10:15 HSZ/0105

Dirac quantum criticality in twisted double bilayer transition metal dichalcogenides — •Jan Biedermann and Lukas Janssen — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

We investigate the phase diagram of twisted double bilayer transition metal dichalcogenides with ABBA stacking as a function of twist angle and pressure. At a filling of 2 holes per moiré unit cell, the noninteracting system hosts a Dirac semimetal with graphene-like low-energy bands. At small twist angles however, interactions dominate the low-temperature physics, stabilizing an antiferromagnetic insulating ground state that is characterized by spin density modulations at the moiré scale. The twist-tuned semimetal-to-antiferromagnet transition is shown to be continuous and belongs to the Gross-Neveu-Heisenberg universality class. We propose that this transition may also be realized by applying uniaxial pressure to a sample, raising the intriguing possibility of experimentally measuring the associated critical exponents for the first time.

HL 14.4 Tue 10:30 HSZ/0105

Chemically Tunable Correlation Strength in Breathing Mode Kagome van der Waals Materials Nb_3(F,Cl,Br,I)$_8$ — •Joost Aretz[1], Sergii Grytsiuk[1], Xiaojing Liu[2], Giovanna Feraco[2], Chrystalla Knekna[2,3], Muhammad Waseem[2], Zhiying Dan[2], Marco Bianchi[4], Philip Hofmann[4], Mazhar Ali[5], Mikhail Katsnelson[1,6], Antonija Grubišić-Čabo[2], Hugo Strand[7], Erik van Loon[8], and Malte Rösner[1,9] — [1]Radboud University, Nijmegen, Netherlands — [2]University of Groningen, Netherlands — [3]University of Amsterdam, Netherlands — [4]Aarhus University, Denmark — [5]Delft University of Technology, Netherlands — [6]Constructor University, Bremen, Germany — [7]Örebro University, Sweden — [8]Lund University, Sweden — [9]Bielefeld University, Germany

Finding tunable correlated electron systems in nature is highly desirable for studying strongly correlated materials. Our recent work demonstrates that the Nb_3X_8-family offers such a platform for tuning correlation effects in van der Waals systems. By using ab initio downfolding and cluster dynamical mean-field theory we show how correlation effects evolve across the halide series. In these materials an intruiging interplay between in-plane trimerization and out-of-plane dimerization leads to correlated insulating behavior, where the strength of correlations can be tuned by switching the halide or by changing the layer number. The predicted trends are supported by ARPES measurements. The correlated electron physics in this system is robust, tunable and layered, which allows studying the role of correlations in devices such as the $NbSe_2/Nb_3Br_8$ Josephson diode.

HL 15: Organic Semiconductors: Optics and Photonics

Time: Tuesday 9:30–12:00 Location: POT/0006

HL 15.1 Tue 9:30 POT/0006

Accessing 'Slow' Dynamics in Photocatalysts with PIAS — •Maria Ferree[1], Rebecca Gröninger[2], Tianhao Xue[1], Thomas Bein[1], Bettina Lotsch[2], and Frédéric Laquai[1] — [1]Dept. Physical Chemistry, LMU München, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Quasi-steady-state Photoinduced Absorption Spectroscopy (PIAS) is a highly sensitive tool for probing long-lived excited states and charge carriers in semiconductors. We showcase PIAS capabilities by studying diverse systems, ranging from conjugated polymers and COF-based films to nanoparticle dispersions. PIAS is often overshadowed as researchers default to sophisticated Transient Absorption (TA) Spectroscopy. However, low-frequency modulated excitation with lock-in signal detection capture extremely weak changes in transmission induced by polarons or triplet states with lifetimes ranging from nanoseconds to seconds - dynamics that remain largely inaccessible by TA, but highly relevant for diffusion-limited processes, e.g. photocatalysis. Frequency-dependent measurements provide insight into lifetimes and concentrations of long-lived species. Whilst Time-resolved Photoluminescence (TRPL) can further reinforce the conclusions obtained from PIAS by extracting exciton recombination kinetics. Our studies of organic semiconductor-based photocatalysts are a reminder that PIAS is a powerful, often more suitable method complementary to ultrafast spectroscopy and other characterisation techniques. It provides unique access to 'slow' excited-state dynamics through relatively straightforward data acquisition and processing.

HL 15.2 Tue 9:45 POT/0006

Subwavelength OLED pixels based on plasmonic electrodes — •Leo Siebigs[1], Cheng Zhang[2], Björn Ewald[1], Luca Steinbrecher[2], Maximilian Rödel[1], Thomas Fleischmann[1], Monika Emmerling[2], Bert Hecht[2], and Jens Pflaum[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg — [2]Experimental Physics 5, University of Würzburg, 97074 Würzburg

Next-generation display technologies, such as augmented and virtual reality, demand the continued miniaturisation of individual pixels. A novel approach towards achieving the necessary ultra-high resolution involves subwavelength organic light-emitting diode (OLED) pixels based on plasmonic nanoelectrodes. The nanoelectrode acts as an optical antenna, ensuring efficient light-outcoupling to the far-field and control over the emission characteristics by adjusting the antenna geometry. However, upon scaling the pixel dimensions below the wavelength of light, sharp nanoelectrode contours dominate the device operation. As a result (i) filament growth leads to rapid device failure and (ii) spatially imbalanced charge-carrier transport and recombination limits the external quantum efficiency (EQE). We address these challenges by selectively passivating the nanoelectrode edges with an insulating layer and defining the active area via a nanoaperture. As proof-of-concept, efficient and stable hole-injection is shown in hole-only devices based on gold nanoelectrodes. For the first time, we demonstrate light extraction from individually addressable 300 nm x 300 nm plasmonic OLED pixels with a maximum luminance of 3000 cd m^{-2} and 1% EQE. C., Zhang et al., Sci. Adv. 2025, DOI: 10.1126/sciadv.adz8579

HL 15.3 Tue 10:00 POT/0006

Near infrared OLEDs for neuroimplants — •Sabina Hillebrandt[1], Sumit Mohapatra[1], Ahmed Gaber Abdelmagid[2], Konstantinos C. Daskalakis[2], Andreas Mischok[1], and Malte C. Gather[1,3,4] — [1]Humboldt Centre for Nano- and Biophotonics, University of Cologne, Germany — [2]Department of Mechanical and Materials Engineering, University of Turku, Finland — [3]School of Physics and Astronomy, University of St Andrews, United Kingdom — [4]CECAD, University of Cologne, Germany

OLEDs offer spectral tunability, mechanical flexibility, and compatibility with scalable thin-film fabrication, making them strong candidates for biointegrated photonic technologies. Near-infrared (NIR) OLED emission can penetrate deep into tissue and may enable neuromodulation without the need for genetic interventions.

We present the development of high-brightness, top-emitting NIR OLEDs specifically engineered for implantable neurotechnology. Using optimized emitter-host combinations, microcavity tuning, and customized charge-transport layers, these devices exhibit peak emission above 800 nm with no measurable output below 700 nm, thereby reducing off-target excitation and tissue scattering. The devices achieve power densities approaching 0.1 mW/mm^2, levels relevant for neuromodulation, while maintaining both thermal stability and robust operational performance. To further refine spectral purity and directional control, we integrate strong-coupling architectures, yielding polariton OLEDs with angular-stable NIR emission above 800 nm even on flexible, implantable polymer substrates.

HL 15.4 Tue 10:15 POT/0006

Aggregation enhanced singlet emission in a purely organic emitter with thermally activated delayed fluorescence — •Jiacheng Gong, Xin Zhou, Kaiwen Guo, Toulik Maitra, Denis Andrienko, Gert-Jan Wetzelaer, Paul W. M. Blom, and Yungui Li — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Purely organic thermally activated delayed fluorescence (TADF) emitters have gained great attentions in the field of organic light-emitting devices. However, the long-lived triplet exciton contributes to efficiency roll-off and device degradation at high current densities. Great efforts have been made to accelerate reverse intersystem crossing (rISC), while there are less studies on the increase of singlet radiative transition rate (krS). Herein, based on the benchmark TADF emitter CzDBA, it is found that it exhibits a larger krS in neat film, which is ~ 4 times faster than that in toluene with similar dielectric environment. The modelling of excited-state dynamics for electrically excited TADF emitters demonstrates that the increased krS reduces triplet and singlet densities simultaneously, while retaining high charge-to-photon conversion efficiency. Furthermore, time-resolved photoluminescence and steady-state absorption spectroscopic analysis shows that the broadened absorption feature increases the oscillator strength and hence increases krS in terms of Strickler-Berg relation. Gaussian disorder model is further applied to PL excitation spectra, and a larger disorder factor from the film samples implies that the large disorder of energetic landscape may contribute to the enhanced krS.

HL 15.5 Tue 10:30 POT/0006

Spectral diffusion of charge-transfer states in organic donor:acceptor blends due to carrier relaxation — •Giacomo Cotelli[1], Anna Köhler[1], and Reinder Coehoorn[2] — [1]University of Bayreuth, Bayreuth, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands

Blends of small-molecule organic semiconductors may display emission from an intermolecular charge transfer (CT) excited state. An aspect that is not well understood so far is the spectral diffusion of such CT states. We present a comprehensive study of CT state spectral diffusion in two- and three-component blends, using kinetic Monte Carlo simulations. We disentangle the effects of the CT state lifetime, charge carrier energetic disorder and blend composition on the emission spectra. Furthermore, we highlight similarities and differences between the emission of photogenerated CT states in films and electrically generated CT states in OLEDs.

HL 15.6 Tue 10:45 POT/0006

Direct Prediction of Organic Light-emitting Diode Efficiency Roll-off from Photophysical Parameters of Thermally Activated Delayed Fluorescence Emitters — •Kaiwen Guo, Yungui Li, and Paul Blom — Max Planck Institute for Polymer Research, Mainz, Germany

Severe efficiency roll-off significantly limits the practical performance of organic light-emitting diodes (OLEDs) at high luminance, especially for the devices based on thermally activated delayed fluorescence (TADF) emitters. Although numerous TADF emitters have been developed and investigated over last decade, in molecular scale the intrinsic molecular-origin of roll-off still remains unclear. In this work, we establish a direct correlation between device roll-off and intrinsic photophysical properties of TADF emitter, and analytically derive the roll-off as a function of exciton generation rate.

We propose an integrated methodology to extract complete set of photophysical parameters of TADF emitter, including the rates of exciton decays, spin conversion kinetics and bimolecular annihilation coefficients. Notably, we reveal that the roll-off behavior in TADF based

OLED is not solely governed by bimolecular annihilation processes, but also influenced by the lifetime of delayed fluorescence. This knowledge enables us to predict the severity of roll-off directly from optical measurements and provides insight for further molecule designing.

15 min. break

HL 15.7 Tue 11:15 POT/0006

OLED-based implants for neurostimulation — •Sumit Mohapatra[1], Falko Fuhrmann[2], Julian F. Butscher[1,3], Sabina Hillebrandt[1,3], Martin Fuhrmann[2], and Malte C. Gather[1,3,4] — [1]Humboldt Centre for Nano- and Biophotonics, Department of Chemistry, University of Cologne, Germany — [2]Neuroimmunology and Imaging Group, DZNE, Bonn, Germany — [3]School of Physics and Astronomy, University of St Andrews, UK — [4]CECAD, University of Cologne, Germany

Light-based neurostimulation allows precise manipulation of neural circuits, yet delivering light to deep tissue remains a challenge. OLEDs combine spectral tunability, mechanical flexibility, and thin-film integration, enabling fabrication of neural probes for localized stimulation.

We advance this approach by integrating OLEDs onto magnetoelectric substrates to create fully wireless neuromodulation platforms, which are 200 μm-thick, contain 300*500 μm^2 OLEDs delivering mean power densities of 0.04 mW/mm^2. Tunable kilohertz-range resonances allow clustered multi-pixel operation, while thin-film encapsulation ensures biocompatibility and protection in a physiological environment. We also introduce a flexible OLED-based neuroprobe by integrating OLEDs onto 15 μm-thick commercial electrophysiology arrays. Using these pre-validated implantable platforms, they are transformed into μOLED arrays with 28 individually addressable μOLEDs (50 μm diameter, 300 μm pitch), achieving power density up to 0.1 mW/mm^2 at 7 V. In vivo optogenetic experiments using μ-OLEDs in mice confirm effective neuronal activation, verified by two-photon calcium imaging.

HL 15.8 Tue 11:30 POT/0006

Exploring Molecular Stability in Organic Solar Cells: A Combined DFT and ML Approach — •Muhammad Waqas and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

The stability of organic solar cells (OSCs) remains a significant challenge in the field. In this work, we present a data-driven approach that integrates density functional theory (DFT) and machine learning (ML) to identify molecular parameters that influence device stability. For this purpose, we compute different optical and electronic parameters by using DFT and time-dependent DFT and check their influence on the lifetime (T80) of OSCs. The first step is to collect lifetime data from the already published literature for different OSC materials. The second step involves DFT and TD-DFT calculations for the selected molecules, thereby generating a dataset. This dataset serves as a foundation for training the ML models. Based on the DFT-generated data, we train ML models that can help us recognise the most influential parameters that affect the stability of OSCs. Furthermore, based on the insights gained from the ML models, we can explore the chemical space to find other molecules that can be used to prepare more stable devices.

HL 15.9 Tue 11:45 POT/0006

Accurate characterization of next-generation photodiodes — Siddhartha Saggar[1,2], Giedrius Puidokas[2], and •Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, 04736 Waldheim, Germany

Photodiodes based on organic and emerging semiconductor materials have demonstrated high potential for optical sensing in biomedicine, imaging applications, and light-based data transmission. During the last decade, concerns have arisen regarding the reliable reporting of the device performance, especially under low illumination conditions. This work addresses these concerns and provides a robust framework for measuring and reporting standardized photodetection metrics. We have developed a measurement setup including a highly sensitive electrometer, calibrated optical filters, and light sources with narrowband emission spectra. For operation of the setup, we provide open-source Python scripts and outline protocols suitable for accurate characterization of steady-state photodetecting metrics.

HL 16: Focus Session: Quantum Emitters in 2D Semiconductors

Quantum emitters are fundamental building blocks in the development of scalable quantum communication networks. They provide capabilities for single-photon generation, quantum memory, and entanglement distribution*essential components for quantum key distribution, quantum repeaters, and future quantum internet infrastructure. Two-dimensional (2D) materials have recently emerged as a highly promising platform for quantum photonics. Their atomically thin nature enables strong light-matter interaction, high tunability, and seamless integration with photonic and electronic environments. Moreover, the reduced dielectric screening and strong excitonic effects inherent to 2D materials provide unique opportunities to engineer and control localized excitonic states that act as quantum emitters. This combination of physical richness and technological compatibility places 2D materials at the frontier between fundamental quantum optics and device-level quantum technologies. To advance the field, it is essential to understand both the microscopic theoretical principles and the engineering challenges associated with integrating such systems into communication networks.

Organized by Michael Lorke, Iris Niehues and Tobias Heindel

Time: Tuesday 9:30–12:45 Location: POT/0081

Invited Talk HL 16.1 Tue 9:30 POT/0081

Tailoring the performance of WSe_2 quantum emitters via cavity quantum electrodynamics and coherent driving — •Ivan Solovev — Institute of Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany

The ability to create scalable arrays of bright and easily-fabricated single photon sources has sparked keen interest in Van der Waals materials, rendering them a promising platform for emerging quantum technologies. Here I will provide an overview how their performance can be substantially improved via integration into a tunable microcavity as well as exploiting resonant excitation schemes. The implementation of the monolithic Fabry-Pérot open cavity, operating in a weak coupling regime, enables the observation of phenomena such as Purcell enhancement of radiative decay, strain-induced tuning of the emitter energy and two-photon interference. An impact of phonons on dephasing and resulting indistinguishability will be discussed. Furthermore, the selective excitation in a coherent manner is achieved via resonant driving, leading to the observation of Rabi oscillations.

Invited Talk HL 16.2 Tue 10:00 POT/0081

Deterministic single-photon emitters in 2D materials — •Ursula Wurstbauer — University of Münster, Germany

Single-photon emitters (SPEs) play a pivotal role as building blocks for quantum technologies. In two-dimensional (2D) materials, SPEs can deterministically be generated, externally manipulated and monolithically integrated. The properties of SPEs in atomically thin membranes are strongly dependent on the host materials and differ e.g. between TMDCs and hBN but also on the emitters origin, like defects, strain or moiré-potentials in twisted structures [1,2]. SPEs can be generated on-demand and on-chip with high lateral precision in the

prototypical TMDC monolayer MoS2 by defect engineering utilizing focused helium ions [3]. These defect states in TMDCs interact with the electronic bands, whereas some defects in hBN show color center like behavior [1]. Following a general introduction, we focus on generation and characterization of rather monoenergetic SPEs in hBN by Argon ion irradiation [4]. We gratefully acknowledge A. R. Bhuiyan, R. Schmidt, A. Michaelis de Vasconcellos, R. Bratschitsch and Harry Mönig for fruitful collaboration. [1] S. Michaelis de Vasconcellos et al. Physica status solidi b259, 2100566 (2022). [2] M. Brotons-Gisbert, et al. MRS Bulletin 49, 914-931 (2024). [3] J. Klein et al. ACS Photonics, 8, 2, 669-677 (2021). [4] A. R. Bhuiyan et al.

Invited Talk HL 16.3 Tue 10:30 POT/0081

Resolving atomic and electronic structure of point defects in MoS_2 by first-principles calculations and scanning tunneling microscopy — •Hannu-Pekka Komsa — University of Oulu, Oulu, Finland

A unique advantage of 2D materials is that the defects in them are always at or very near to the surface, which can be highly beneficial in quantum emitter and quantum sensing applications. Importantly, this also enables direct characterization and manipulation of the defects with surface-sensitive techniques, such as scanning tunneling microscopy (STM). Since STM probes mainly the electronic structure, defect identification often requires comparison to results from first-principles calculations.

I will present our recent investigations on the electronic structure of a few common point defects in 2D MoS_2, such as S vacancies, Mo and Fe adatoms, and C substitutional on S site, combining first-principles calculations and experimental STM results from University of Cologne and Karlsruhe Institute of Technology. I will first discuss the computational aspects that were found to be important in achieving good agreement with experiments. A careful analysis and comparison of the computational and experimental results then allow us to infer defect identity, charge state, defect-defect interactions, magnetic moment, and dynamic effects such as defect transformations among Jahn-Teller configurations, defect charging, and spin lifetimes. Finally, benefiting from the atomic manipulations inside STM, rational atom-by-atom fabrication of defect structures can be envisioned.

15 min. break

Invited Talk HL 16.4 Tue 11:15 POT/0081

Polarization dynamics of isolated defects in hexagonal boron nitride — Serkan Paçal[1], Çağlar Samaner[1], Furkan Ağlarcı[1], Ömer S. Tapşın[1], and •Serkan Ateş[1,2] — [1]Department of Physics, Izmir Institute of Technology, Izmir, Turkey — [2]Faculty of Engineering and Natural Science, Sabanci University, Istanbul, Turkey

Single-photon sources (SPSs) are indispensable for quantum information technologies like Quantum Key Distribution. The practical success of these applications critically depends on the high purity and long-term stability of the emitted light's polarization state, which serves as the information-carrying quantum bit (qubit). Understanding and controlling polarization dynamics, therefore, presents a universal challenge for establishing reliable solid-state quantum interfaces. We propose using hexagonal Boron Nitride (hBN) defect centers as a promising new platform for SPSs exhibiting strong, stable single-photon emission at room temperature, making it an ideal model system. In this work, we specifically investigate the polarization properties of hBN defect centers. We analyze the dynamics and temperature dependence of the polarization degree, focusing on the influence of electron-phonon interactions. Our results offer crucial insights that enable the development of targeted strategies to enhance the polarization stability of single-photon emitters, thereby facilitating more robust quantum optical systems.

Invited Talk HL 16.5 Tue 11:45 POT/0081

Defect-driven quantum emission in 2D materials — •Magdalena Grzeszczyk — IFIM, NUS, 117544, Singapore

Carbon-doped hexagonal boron nitride (hBN:C) provides a compelling 2D analogue to classical wide-bandgap hosts such as ruby (Cr:Al2O3), where isolated impurity centers give rise to sharp, stable optical transitions. These point defects have emerged as robust and manipulatable single-photon emitters (SPEs). By combining a broad suite of experimental techniques with advanced theoretical modeling, we introduce a consistent assignment of the observed excitations in hBN:C to the most likely underlying defect complexes. The described defect states residing in close proximity to the surface present an ideal sensors of local fields at the nanoscale. An example of how the local dielectric environment strongly modulates these centers, producing distinct spectral shifts will be discussed. Additionally, these defect states can be electrically excited in hBN-based light-emitting diode structures, providing a route toward integrated quantum emitters in van der Waals devices. Finally, ZnPS3 will be introduced as an emerging new host of SPEs. As a representative member of a broader family of layered MPX3 compounds, such as MnPS3 and FePS3, this emergent host opens new platform for future exploration of SPEs with intrinsic magnetic tunability.

HL 16.6 Tue 12:15 POT/0081

Nanoscale magnetic field sensing with spin defects in hexagonal boron nitride — •Korbinian Felber, Timo Strobl, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, Julius-Maximilians-Universität Würzburg (JMU), 97074 Würzburg, Germany

The development of quantum sensors based on solid-state spin defects is a vibrant research area, yet most host materials are three-dimensional, making it challenging to position the sensing spins in close proximity to a target sample. This limitation was recently overcome in 2020 with the discovery of the negatively charged boron vacancy (V_B^-) in the two-dimensional van der Waals material hexagonal boron nitride (hBN). Exfoliating spin-active hBN flakes provide coherent spin manipulation in an atomically thin host. Using optically detected magnetic resonance (ODMR), these hBN spin defects provide sensitive readout of local magnetic fields, temperature, and strain, making functional hBN layers an ideal platform for exploring fundamental questions in 2D magnetism. In this study, we assemble a vdW heterostructure by stacking active hBN on top of a 2D ferromagnet. By employing spin-relaxometry techniques, we probe nanoscale magnetic fluctuations near the Curie temperature of the exfoliated ferromagnet. Our results highlight the potential of hBN-based quantum sensors for characterizing local magnetic properties in vdW heterostructures, offering substantial benefits for the design of next-generation 2D devices.

HL 16.7 Tue 12:30 POT/0081

Ion-beam induced quantum emitters in hexagonal boron nitride — •Jan Böhmer, Annkathrin Köhler, Hannes Simon, Lucas Böhme, and Carsten Ronning — Friedrich Schiller University, Jena, Germany

Defect centers in solid-state materials are emerging as highly promising candidates for realizing robust quantum light sources. Among these, hexagonal boron nitride (hBN) has attracted significant interest due to its potential for hosting room-temperature single photon emitters (SPEs). We utilize ion-beam irradiation to introduce optically active defect centers into hBN, offering a controlled and tunable method for engineering defect centers. We have investigated intrinsic and extrinsic ion-beam induced defect centers in exfoliated hBN flakes: Microphotoluminescence spectroscopy (μ-PL) was employed to characterize the spectral properties of the induced emitters, while second-order correlation measurements ($g^{(2)}$) were performed to demonstrate the single-photon emission behavior and determine the quantum nature of the sources. Additionally, in-situ electrical measurements were used to monitor the reaction of the hBN flakes to irradiation in real-time. The results demonstrate that ion-beam irradiation can be successfully utilized for creation of quantum emitters in hBN. This work contributes to the ongoing effort to develop reliable, solid-state single photon emitters for quantum applications.

HL 17: Quantum Dots and Wires: Rings, Wires and Transport

Time: Tuesday 9:30–12:15 Location: POT/0251

HL 17.1 Tue 9:30 POT/0251

Growth of hexagonal Silicon Germanium quantum rings — •Marvin Marco Jansen[1], Mette F. Schouten[1], Denny Lamon[1], Wouter H.J. Peeters[1], Marcel A. Verheijen[1,2], and Erik P.A.M. Bakkers[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherlands — [2]Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands

Developing a silicon-based laser represents a key step toward commercially viable photonic circuits. A promising route is the recently discovered hexagonal silicon germanium (hex-SiGe) grown as shells around gallium arsenide (GaAs) nanowires (NWs), which has demonstrated efficient direct band-gap emission. In addition, type-I band alignment was demonstrated in hex-SiGe/Ge quantum wells (QWs), pushing the system closer to lasing. Theory predicts that combining hexagonal/cubic Ge(Si) QWs could further enhance optical performance. Here, we investigate the growth of hex-SiGe/Ge QWs on GaAs NWs that alternate between wurtzite (WZ) and zinc blende (ZB) crystal phases, forming ring-shaped hexagonal Ge QWs. These quantum rings feature two types of confinement: crystal-phase-induced axial confinement and radially controlled alloy composition. We explore several different WZ/ZB superlattice designs and TEM analysis confirms successful integration of hexagonal/cubic SiGe alloys and SiGe/Ge QW shells on the designed superlattices. Our results establish crystal-phase superlattice NWs as a promising platform realizing hex-Ge quantum rings and marking progress towards a hex-SiGe laser.

HL 17.2 Tue 9:45 POT/0251

A road to parallelisation - spin qubits as single electron pumps — •Dustin Wittbrodt[1], Johannes Christian Bayer[1], Lars Schreiber[2], Janne Lehtinen[3], and Frank Hohls[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]JARA Institute for Quantum Information, Forschungzentrum Juelich, Germany — [3]SemiQon Technologies Oy, Espoo, Finland

The main workhorse of low current Ampere realization is the Single Electron Pump (SEP), which generates quantized currents based on the quantized transport of single charge carriers. The result are currents in the fA-pA range, measureable with a precision of as low as 0.1 ppm. For further improvement of accuracy and current output, parallelization of pumps is the necessary next step. Semiconductor spin qubit devices offer an interesting solution. In addition to sharing the same central building unit, the quantum dots, spin qubits also offer the possibility of incorporating CMOS logic and taking advantage of a mature, high-yield industry for large scale SEP manufacturing, thus allowing for the implementation of a high number of pumps with minimal control inputs. Various Si and Si-compound spin qubit technology platforms are being tested as SEP candidates, within the EU-funded AQuanTEC project. The focus of the activities includes the characterisation of these spin qubits in DC measurements and then in a series of AC measurements to characterise the pumping behaviour of these devices. We present the results of this effort here, offering a perspective on the potential application of Qubit technology for broader use as quantum metrological instruments.

HL 17.3 Tue 10:00 POT/0251

Using full counting statistics to identify interactions in the electron dynamics in a self assembled quantum dot — •Johann Zöllner, Hendrik Mannel, Daniel Oppers, Axel Lorke, Martin Geller, and Jürgen König — Faculty of Physics and CENIDE, University of Duisburg-Essen

We study interactions and electron dynamics in a self-assembled quantum dot using full counting statistics. Each tunneling event identified with a resonance-fluorescence-based continuous measurement [1]. Full counting statistics provides much more information than just the average current through the system. The details of the probability distribution obtained from full counting statistics depends on whether interactions play a role in electron transport or whether it can be modeled by noninteracting fermions [2,3]. This is reflected in sign changes of the factorial cumulants calculated from the probability distribution. Factorial cumulants are a measure for fluctuations and are particularly suited to characterize discrete distributions. We identify these sign changes predicted by theory in the experimental data. In this way, simply by observing individual tunneling events between the dot and a reservoir, we have gained information about the electron dynamiks like spin relaxation between Zeeman-split energy level and the presence of interactions.

[1] A. Kurzmann *et al.*, PRL **122**, 247403 (2019)
[2] D. Kambly *et al.*, PRB **83**, 075432 (2011)
[3] P. Stegmann *et al.*, PRB **92**, 155413 (2015)

HL 17.4 Tue 10:15 POT/0251

Effective Hamiltonians for Ge/Si core/shell nanowires from higher-order perturbation theory — Sebastian Miles[1], A. Mert Bozkurt[1], •Dániel Varjas[2,3,4], and Michael Wimmer[1] — [1]QuTech and Kavli Institute of Nanoscience, Delft University of Technology — [2]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Max Planck Institute for the Physics of Complex Systems — [4]Budapest University of Technology and Economics

We theoretically explore the electronic structure of holes in cylindrical Germanium/Silicon core/shell nanowires using a perturbation theory approach. The approach yields a set of interpretable and transferable effective low-energy model parameters for the lowest few sub-bands up to fifth order in perturbation theory for various experimentally relevant growth directions. In particular, we are able to resolve higher-order cross terms, e.g., the dependency of the effective mass on the magnetic field. Our study reveals orbital inversions of the lowest sub-bands for low-symmetry growth directions, leading to significant changes of the lower order effective coefficients. We demonstrate a reduction of the direct Rashba spin-orbit interaction due to competing symmetry effects for low-symmetry growth directions. Finally, we find that the effective mass of the confined holes can diverge, yielding quasi flat bands interesting for correlated states. We show how one can tune the effective mass of a single spin band allowing one to tune the effective mass selectively to its divergent points.

HL 17.5 Tue 10:30 POT/0251

Improving optical quality in highly strained GaAs/$In_xAl_{1-x}As$ core/shell nanowires — Xiaoxiao Sun, •Alexej Pashkin, René Hübner, Finn Moebus, Yuxuan Sun, Andreas Worbs, Slawomir Prucnal, Shengqiang Zhou, Stephan Winnerl, Manfred Helm, and Emmanouil Dimakis — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

III-V semiconductor nanowires are promising for applications in photonics, electronics, and sensing. In lattice-mismatched GaAs/$In_xAl_{1-x}As$ core/shell nanowires, tensile strain in the GaAs core enables substantial bandgap tuning across the near-infrared spectrum. However, $In_xAl_{1-x}As$ shells are typically grown at low temperatures, which compromises their structural quality and induces non-radiative recombination. We present two strategies to mitigate it. The first employs a dual-shell architecture in which an intermediate $Al_yGa_{1-y}As$ shell spatially separates carriers in the GaAs core from the $In_xAl_{1-x}As$ shell [1]. Optimizing the spacer thickness significantly enhances photoluminescence efficiency and extends emission lifetimes. The second strategy focuses on optimizing the shell growth conditions. We show that higher growth temperatures improve the core/shell interface quality, reducing non-radiative recombination and carrier scattering, with optimal performance near 500°C [2]. This allows a simple single-shell structure to approach the performance of the more complex dual-shell design.

[1] X. Sun et al., *Adv. Funct. Mater.* **34**, 2400883 (2024).
[2] X. Sun et al., *Appl. Phys. Lett.* **127**, 182107 (2025).

HL 17.6 Tue 10:45 POT/0251

Quantum dot as a model system for a Hund's coupled impurity — •Olfa Dani[1], Johannes C. Bayer[1,2], Timo Wagner[1], Gertrud Zwicknagl[3], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany

In this work, we investigate electron transport through the third shell [1] of a gate-defined GaAs quantum dot, where the exact electron number (N) is determined using a quantum point contact and tuned in a controlled manner by changing the applied gate voltages of the device

[2]. For N = 7-11, the addition energy shows a triangular evolution with a maximum at half-filling. This trend is reproduced by model calculations including Hund's rule exchange. In the same filling range, a zero-bias anomaly (ZBA) characteristic of the Kondo effect appears. Its width and amplitude display a similar triangular dependence, reflecting the particle-hole symmetry of the three spin-degenerate orbitals. The pronounced ZBA is attributed to the contribution of both the Kondo resonance and low-energy Hund satellite excitations associated with degenerate orbitals observed in the spectral function [3]. The quantum dot is viewed as a multi-orbital Kondo impurity with Hund's interaction and serves as a model system for a Hund's coupled impurity. [1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64 (2001). [2] T. Wagner, et. al., Nat. Phys.15 (2019). [3] O. Dani, et. al., arXiv: 2505.21675 (2025).

15 min. break

HL 17.7 Tue 11:15 POT/0251

Quantum stochastic resonance in a single-photon emitter — •H. Mannel[1], J. Zöllner[1], E. Kleinherbers[2], M. Zöllner[1], N. Schwarz[1], F. Rimek[1], A. Ludwig[3], A. Lorke[1], J. König[1], and M. Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Classical stochastic resonance (SR) describes how noise can enhance the response of a driven bistable system. Recently, it has been extended to the quantum regime, where fluctuations originate from single tunneling events [1]. Building on optical real-time charge detection in self-assembled quantum dots [2], we demonstrate quantum stochastic resonance in a single InAs/GaAs quantum dot, weakly tunnel-coupled to an electron reservoir. Periodic modulation of the gate voltage synchronizes the electron tunneling with the external drive, while resonance fluorescence provides a fully optical, high-resolution readout of the charge state. From the full counting statistics of the tunneling events, we observe a pronounced narrowing of the distribution at the resonance condition, marking the transition from stochastic to increasingly deterministic transport [3]. [1] T. Wagner et al., Nat. Phys. 15, 330 (2019). [2] A. Kurzmann et al., Phys. Rev. Lett. 122, 247403 (2019). [3] H. Mannel et al., Commun Phys 8, 404 (2025).

HL 17.8 Tue 11:30 POT/0251

Spin relaxation dynamics of the excited triplet state in self-assembeld quantum dots — •Carl Nelson Creutzburg[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 self-assembled quantum dots (QDs) can pair with the singlet ground state to form an electrically addressable spin qubit candidate. Using such qubits for quantum information processing requires long coherence times T_2, ultimately limited by the spin relaxation time T_1. While T_1 has predominantly been probed using optical techniques, we here present an all-electrical approach to access the spin relaxation dynamics.
The QDs are embedded in an inverted high-electron-mobility transistor, allowing controlled electron tunneling between the dots and a coupled two-dimensional electron gas (2DEG), which also serves as a sensitive charge detector. Using time-resolved transconductance spectroscopy [1] with a three-level pulse sequence, we observe the relaxation from the excited triplet to the singlet state as a function of the charging interval. A rate-equation analysis yields the spin relaxation time T_1. This approach provides an independent and complementary route to previous studies [2] and may help refine key assumptions.
[1] B. Marquardt et al., Nature Commun. 2, 209 (2011)
[2] K. Eltrudis et al., Appl. Phys. Lett. 111, 092103 (2017)

HL 17.9 Tue 11:45 POT/0251

CMOS Compatible Short-Channel Junctionless Nanowire Transistors — •Sayantan Ghosh[1,2], Alessandro Puddu[1,2], Slawomir Prucnal[1], Yordan M. Georgiev[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany

The demand for miniaturized, high-speed, and energy-efficient electronics is pushing conventional planar transistors to their scaling limits, where short-channel effects and fabrication complexity constrain performance. Junctionless nanowire transistors (JNTs) offer a promising alternative through simplified architecture, strong electrostatic control, and CMOS compatibility. Using uniformly doped channels and eliminating pn-junctions, JNTs reduce process complexity and improve scalability for next-generation nanoelectronics. In this work, short-channel silicon JNTs were fabricated on SOI substrates using a CMOS-compatible top-down method. The devices use 20 nm-wide n-type Si nanowires with channel lengths from 1000 nm to 50 nm. Back-gate operation shows clear ambipolar behaviour, while top-gate operation yields the unipolar response characteristic of true JNTs. The 50 nm device achieves a current on/off ratio > 5 orders of magnitude and a subthreshold swing of around 200 mV/dec, demonstrating strong potential for low-power nanoscale technologies.

HL 17.10 Tue 12:00 POT/0251

Majorana bound states in 1D superconducting nanowires: detection, transport, and braiding — •Suhas Gangadharaiah — Indian Institute of Science Education and Research Bhopal India

Majorana bound states (MBSs) have emerged as promising candidates for robust quantum computation due to their topological protection. However, similar tunneling conductance features for both the MBSs and certain types of Andreev bound states have turned out to be a major obstacle in the verification of the presence of MBSs in semiconductor-superconductor heterostructures. In this talk, we will first discuss our protocol to probe properties specific to the MBSs and use it to distinguish the topological zero-bias peak (ZBP) from a trivial one [1]. We will next consider the dynamical transport of MBSs in the semiconductor-superconductor heterostructure in a realistic scenario involving noisy conditions and their role in inducing diabatic errors. We will discuss the scaling laws that relate these errors to the drive time [2]. Finally, we will discuss our ongoing work on MBS braiding in a trijunction geometry composed of three connected Kitaev chains.
1. Dibyajyoti Sahu, Vipin Khade, and Suhas Gangadharaiah. Effect of topological length on bound state signatures in a topological nanowire. Phys. Rev. B, 108:205426, Nov 2023.
2. Dibyajyoti Sahu and Suhas Gangadharaiah. Transport of Majorana bound states in the presence of telegraph noise. Physical Review B, 111(23):235306, June 2025.

HL 18: Nanomechanical systems (joint session HL/TT)

Time: Tuesday 10:00–12:45 Location: POT/0051

HL 18.1 Tue 10:00 POT/0051

Mechanical characterization of freely-suspended crystalline YIG nanodevices — •Jonny Qiu[1,2], Matthias Grammer[4,5], Sebastian Sailler[6], Sebastian T. B. Goennenwein[6], Michaela Lammel[6], Hans Huebl[3,4,5], and Eva Weig[1,2,3] — [1]TUM School of Computation, Information and Technology, Garching, Germany — [2]Zentrum für Quantum Engineering, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]TUM School of Natural Sciences, Garching, Germany — [5]Walther-Meißner-Institut, BAdW, Garching, Germany — [6]University of Konstanz, Department of Physics, Konstanz, Germany

Efficient quantum transduction, the reciprocal conversion of quantum signals from one energy level to another, is an ongoing challenge in quantum network applications. Engelhardt et al. [1] proposed a microwave to optical converter (MWOC) that co-localizes microwave, magnetic and elastic excitations within a suspended optomechanical crystal (OMC) made of crystalline yttrium iron garnet (YIG).

In this talk, we report our progress towards realizing the MWOC and present freely-suspended YIG nanodevices. We fabricated YIG cantilevers and beams using an electron beam lithography process and a subsequent crystallization by annealing approach. Piezo-driven interferometric spectroscopy reveals the mechanical response modes of these devices, from which we extract Young's modulus and internal stress to design the OMC as a MWOC. We visualize and thus confirm the corresponding mode shapes via laser doppler vibrometry.

[1] F. Engelhardt, et al., Phys. Rev. Appl. 18, 044059 (2022).

HL 18.2 Tue 10:15 POT/0051

Sensing local temperature changes of a silicon nitride nanomembrane under large-amplitude vibration — •Valentin Barth, Mengqi Fu, and Elke Scheer — University of Konstanz, Konstanz, Germany

In MEMS and NEMS, changes in environmental conditions (e.g., a global change in temperature [1]) can alter the motion properties of silicon nitride (SiN) membranes. Vibrational motion may cause the membrane to experience local heating effects.

SiN square membranes (side length: 450 μm, thickness: 500 nm) are used and driven with a piezoelectric actuator. The motion is monitored using digital holographic microscopy. The measurements are carried out with a strong drive, resulting in vibration amplitudes on the order of hundreds of nanometers. Local temperatures are measured via the Seebeck effect using permalloy ($Ni_{81}Fe_{19}$) and gold as thermocouple, which provides a sensitivity of 20 μV/K and is suitable for micrometer-scale measurements [2]. To improve the signal-to-noise ratio and suppress unwanted contributions, the measurement is performed with a lock-in amplifier, where the temperature signal is demodulated at twice the drive frequency. The measured temperature depends on both the position of the thermometer and the vibration amplitude, with values reaching up to 0.5 mK. Besides the temperature signal of the membrane, signals caused by vibrations from neighboring membranes (distanced 1.5 mm) are also detected.

[1] F. Yang et al., Sens. Actuators A Phys. 354, 114307 (2023).
[2] F. L. Bakker et al., J. Appl. Phys. 111, 084509, (2012)

HL 18.3 Tue 10:30 POT/0051

FEBID and FIBID nanowire field emitters integrated with microcantilevers - fabrication and characterization — •Ewelina Gacka[1,2], Gregor Hlawacek[1], Krzysztof Kwoka[2], Tomasz Piasecki[2], Bartosz Pruchnik[2], René Hübner[1], and Teodor Gotszalk[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Department of Nanometrology, Wroclaw University of Science and Technology, 50-370, Wroclaw, Poland

Because micro- and nanomechanical systems are continuously evolving, there is a need to leverage various fabrication technologies. A scanning electron microscope with a gallium focused ion beam, as well as a helium ion microscope, were used to integrate platinum-carbon (Pt-C) and tungsten-carbon (W-C) nanowire field emitters with microcantilevers, serving as deflection sensors. Pt-C and W-C nanocomponents were fabricated using an additive, direct-writing method - focused-electron-/ion-beam-induced deposition (FEBID/FIBID)[1,2]. After growth calibration, the field emission behavior was studied in situ inside a vacuum chamber. The deposited Pt-C and W-C materials were characterized using Kelvin probe force microscopy and transmission electron microscopy. [1] T. Piasecki et al., Nanotechnology 35 (2024), doi: 10.1088/1361-6528/ad13c0. [2] E. Gacka et al., Measurement 234 (2024), doi: 10.1016/j.measurement.2024.114815.

HL 18.4 Tue 10:45 POT/0051

Optimization of Faraday Cage Angled Etching and Its Application Prospects in Silicon Carbide — •Wuzheng Ge[1,2], Ciaran Fowley[1], Jens Zscharschuch[1], Claudia Neisser[1], Artur Erbe[1,2], Philipp Bredol[3], Felix David[3], and Eva Weig[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Dresden University of Technology, Faculty of Electrical and Computer Engineering, 01069 Dresden, Germany — [3]Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

This work presents the optimization of a Faraday Cage Angled Etching (FCAE) approach for ICP-RIE. By reshaping the plasma potential through the cage's mesh geometry, FCAE steers ions along the cage-wall normal, enabling controllable ion incidence angles. Reproducible 3D triangular cross-section structures were demonstrated on silicon, confirming the effectiveness of ion-direction tuning. The results were also applied to silicon carbide nanomechanical resonators. The enhanced directional ion flux enables direct fabrication of free-standing, stress-free structures in bulk, undoped SiC. This capability offers new pathways for advanced SiC-based MEMS.

15 min. break

HL 18.5 Tue 11:15 POT/0051

Probing Mechanical Nonlinearities with Quantum Dots — •Noah Spitzner, Jona Richter, Emeline Denise Sophie Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Münster, Germany

The coupling of quantum dots to mechanical resonances is a well-established approach to investigate the behaviour of mechanical resonators and crystals. Within that approach, the quantum dots (QDs) act as point-like sensors sensitive to dynamical changes to their lattice constant. Vibrations in the host structure modulate the emission energy of the quantum dot, enabling readout of mechanical modes via ultrafast optical detectors. In our hybrid structures, mechanical excitation is achieved by integrating the QD-membrane onto a lithium niobate substrate equipped with finger-like electrodes called interdigitated transducers (IDTs). Applying a radio-frequency (RF) signal to the IDTs generates surface acoustic waves, which propagate on the surface of the substrate, coupling to quantum dots in their path.

This hybrid platform was taken a step further by structuring the QD-membrane into rings hosting mechanical resonances. Frequency sweeps of the RF signal applied to the IDT revealed sharp resonances in the emission-energy modulation exclusively for the quantum dots located within the rings. Interestingly, the resonances appear over a large region of SAW frequencies from 200 MHz to 900 MHz. Moreover, we detect clear signatures of a nonlinear mechanical response e.g. asymmetric lineshapes in the time-modulated optical signal of the QD when the external drive by the IDT is increased.

HL 18.6 Tue 11:30 POT/0051

Dry processing of 3C-silicon carbide nanostring resonators — •Felix David[1,2,3], Yannick Klass[1], Philipp Bredol[1,2,3], and Eva Weig[1,2,3] — [1]Technische Universität München, School of Computation, Information and Technology, Garching, Germany — [2]Technische Universität München, Zentrum für QuantumEngineering (ZQE), Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. In conventional fabrication processes, electron-beam lithography with PMMA is employed to define a metallic hard mask for the subsequent dry etching step via a liftoff process. This requires some wet-chemical process steps, such as HF etching and metal removal, which can destroy samples. Here, we describe an alternative process that avoids all wet-chemical process steps, enabling 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 its high reliability, combined with high process speed, it also allows for quick adaptation to new projects, such as multilayer and hybrid mechanical systems.

HL 18.7 Tue 11:45 POT/0051

The best of two worlds: hexagonal boron nitride exfoliated on stressed silicon carbide string resonators — •Philipp Bredol[1], Felix David[1], Junhui Wu[2], Andrey N. Anisimov[2], Takashi Taniguchi[3], Kenji Watanabe[3], Georgy V. Astakhov[2], Artur Erbe[2], and Eva M. Weig[1] — [1]TU Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany — [2]HZDR, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The boron vacancy (VB) of hexagonal boron nitride (h-BN) is a promising single photon emitter for applications in quantum technologies. Nanomechanical control of the VB would greatly enhance its versatility in such applications, therefore nanomechanical h-BN resonators are of great interest. Here we demonstrate that h-BN can be exfoliated on a chip with a pre-stressed silicon carbide thin-film and subsequently patterned into nanomechanical string resonators with high tensile stress. The resulting h-BN covered string resonators have high mechanical quality factors due to dissipation dilution and show the optically detected magnetic resonance signature of the VB of h-BN. Our fabrication approach allows to decouple the choice of the defect hosting 2D-material from the engineering of the mechanical mode and paves the way to nanomechanical control of single photon emitters in h-BN and other 2D materials.

HL 18.8 Tue 12:00 POT/0051

Cavity optomechanics with van der Waals materials — •Aloysius Farrel[1,3], Lukas Schleicher[1,3], Irene Sánchez Arribas[1,3], Leonard Geilen[2,3], Alexander Musta[2,3], Alexander Holleitner[2,3], and Eva Weig[1,3] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Walter Schottky Institute, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Freely suspended two-dimensional materials are promising platforms for hybrid quantum systems that combine mechanical, optical, and electronic properties. Coupling the optical and mechanical modes of the resonators would be the first step towards such hybrid quantum system.

Here, we present studies of the mechanical resonators with van der Waals materials, such as hBN, on a SiN membrane. We map the spatial mechanical modes of the freestanding and supported 2D materials. Furthermore, we observe an optical nonlinearity in our high-finesse fiber optic cavity setup, which could couple to the mechanical modes. This result helps us understand the optomechanical coupling of the system and leads the way for a hybrid quantum device by incorporating quantum emitters in the system.

HL 18.9 Tue 12:15 POT/0051

Imaging GHz surface acoustic waves in epitaxial graphene cavities — •Mingyun Yuan[1], Alberto Hernández-Mínguez[1], Yi-Ting Liou[2], Jens Herfort[1], Joao M. J. Lopes[1], and Paulo V. Santos[1] — [1]Paul-Drude-Institut, Leibniz Institut im Forschungsverbund e.V., Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The imaging of sound has fascinated scientists and the public alike, dating back to Chladni's demonstrations in the 19th century. Nowadays, it is possible to image mechanical vibrations at the nanoscale, enabling direct probing of propagation, scattering and diffraction for high-frequency acoustic waves with short wavelengths. Here, we present the imaging of GHz surface acoustic waves (SAWs) in an epitaxial monolayer graphene nanostructure, based on thermal decomposition of SiC, using atomic-force microscopy (AFM). We observe a near-perfect strain transfer that gives rise to rich acoustic patterns in the phononic cavity formed by the graphene nanostructure. Furthermore, the enhanced acoustic intensity in the graphene region indicates a waveguiding effect, with graphene serving as an atomically thin, embedded shorting layer. Within the cavity, signatures of quantum chaos are observed. The high spatial resolution of AFM enables the investigation of SAW strain transferred onto 2D materials with high precision. The results also demonstrate an epitaxial nanophononic platform for both functional acoustic devices and fundamental studies of quantum phenomena.

HL 18.10 Tue 12:30 POT/0051

Nonlinear vibrational dynamics locally probed by time-resolved electron diffraction — •Kai Nettersheim[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Nonlinear dynamics of micro- and nanoscale electro-mechanical systems can be observed using electrical or optical methods. However, these approaches are often limited in their spatial resolution, which leaves the underlying mechanics only partially accessible. Recent advances in ultrafast electron microscopy (UTEM) enable the highly localized probing of nanoscale oscillators, allowing to retrieve detailed information about their atomic structure and material defects.

Utilizing stroboscopic UTEM imaging techniques, we present the characterization of nonlinear mode dynamics in free-standing silicon membranes employing an event-based electron detector with nanosecond temporal resolution [1]. The high-Q resonator is excited using an optical pulse train driving the sample into the nonlinear regime. Due to the use of event-based converged electron beam diffraction (CBED), phase-accurate measurements of the nanoscale structural motion are provided. Whereas at weak driving, the oscillator displays a simple Duffing-type bistability, higher harmonic overtones as well as period doubling dynamics emerge at higher driving amplitudes.

[1] A. Schröder et al., Ultramicroscopy 256, 113881 (2024)

HL 19: Graphene: Growth, structure and substrate interaction (joint session O/HL)

Time: Tuesday 10:30–12:30 Location: HSZ/0201

Invited Talk HL 19.1 Tue 10:30 HSZ/0201

During-synthesis functionalization of graphene layers — •Cristina Africh — CNR-IOM, Trieste, Italy

Introducing heteroatoms into graphene is a powerful way to modulate its catalytic, electronic, and magnetic properties. During the last decade, we developed a clean and scalable functionalization strategy that exploits the sponge-like properties of nickel substrates as well as the catalytic role played by transition metal (TM) single atoms at graphene edges during Chemical Vapor Deposition synthesis [1]. Following this route, it is possible to grow N-doped, B-doped and TM-doped graphene as well as co-doped layers [2,3,4]. The potential of the functionalized networks for sensing and, as a perspective, for catalysis, was evaluated by monitoring their response upon gas exposure [5,6].

[1] C. Africh, M. Peressi and G. Comelli, Surf. Sci. 753, 122652 (2025). [2] S. Fiori et al., Carbon 171, 704-710 (2021). [3] S. Patil et al., Surf. Interfaces 51, 104700 (2024). [4] V. Chesnyak et al., Sci. Adv. 10, eado8956 (2024). [5] D. Perilli, S. Fiori et al., J. Phys. Chem. Lett. 11 8887-8892 (2020). [6] D. Perilli, V. Chesnyak et al., Angew. Chem. Int. Ed. 64, e202421757 (2025).

HL 19.2 Tue 11:00 HSZ/0201

Heterotriangulene Kagome Graphene Films: Growth and Effect of Kinetic Reaction Parameters — •Wyatt Behn[1], Simon Briesenick[1], Chang Wan Kang[2], Manuel González-Lastre[3], Pablo Pou[3], Rubén Pérez[3], Dmytro Perepichka[2], and Peter Grutter[1] — [1]Dept. of Physics, McGill — [2]Dept. of Chemistry, McGill — [3]Universidad Autónoma de Madrid

Nanoporous graphenes featuring Kagome lattices formed by heterotriangulene units continue to attract interest for their correlated electronic properties. Their symmetry gives rise to flat bands and Dirac cones [1,2]. Covalent organic frameworks (COFs) like these are often synthesized by surface-assisted Ullmann coupling, and are susceptible to defects such as voids, irregular-sided linkages, and limited grain sizes of around 100 nm [3,4]. We perform a series of polymerizations over a range of sample temperatures (180-250 C) for tribromo- and

triiodotrioxaazatriangulene precursors on the Au(111) surface. Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) we interrogate how deposition conditions and choice of halogen affect the final polymer film quality, which we quantify using minimum spanning tree and persistent homology approaches. We also investigate the prevalence of halogenated edge terminations and of undesired organometallic intermediates. Experimental results are complemented by simulated STM and nc-AFM analyses. [1] C. Steiner, et al. Nat. Commun. 8, 14765 (2017). [2] G. Galeotti, et al. Nat. Mater. 19 (2020). [3] M. Lackinger, Chem. Commun. 53 7872 (2017). [4] T. Qin, et al. Commun. Chem. 7 154 (2024).

HL 19.3 Tue 11:15 HSZ/0201

Defect-Driven Formation of Distinct 2D-Ag Phases at the Graphene/SiC Interface — •Sawani Datta[1], Boyang Zheng[2], Arpit Jain[2], Vibha Reddy[1], Kathrin Küster[1], Joshua A. Robinson[2], Vincent H. Crespi[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalation of two-dimensional (2D) materials at the graphene/SiC interface is important for improving environmental stability of the intercalant and tuning graphene's electronic properties. However, the underlying mechanisms remain complex and are still not fully understood. In this study, we show that by modifying the intercalation process, specifically through defect engineering, it is possible to selectively stabilize two distinct phases of intercalated silver (Ag). The previously established phase (Ag_1) aligns with nearly (1×1) registry of SiC [1, 2], while the second phase (Ag_2) develops a denser $(3\sqrt{3}\times3\sqrt{3})R30°$ superstructure on a (5×5) SiC unit cell, producing a 6.25×6.25 Moiré pattern with respect to graphene, as seen in the low energy diffraction (LEED) pattern [2]. Angle-resolved photoemission spectroscopy (ARPES) reveals a striking kaleidoscopic modulation of the Ag_2 and graphene bands, absent in Ag_1, along with notable differences in charge transfer between the two phases. These results demonstrate that defect-controlled, phase-selective intercalation offers a promising pathway to design and explore exotic 2D electronic states at graphene/SiC interfaces. [1] PRB 101, 201407(R) (2020). [2] arXiv:2511.07151v1 (2025).

HL 19.4 Tue 11:30 HSZ/0201

Strain-Induced 2D Pb phases confined between graphene and SiC — •Sergii Sologub[1,2], Markus Gruschwitz[1], Zamin Mamiev[1], Chitran Ghosal[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The intercalation of metals beneath graphene offers a powerful route to stabilizing and protecting novel 2D phases. We performed a detailed intercalation study of Pb beneath the ZLG on SiC(0001) using low-energy electron diffraction (at the temperatures from 70 to 600° C) as well as scanning electron and tunneling microscopy [1]. Our analysis reveals the formation of different 2D Pb monolayer phases, such as stripes and hexagons, which emerge due to the interplay between substrate pinning and strain within the Pb layer, depending on local coverage. The interface reconstruction of Pb was shown can be tuned by varying the details of the intercalation protocol. Based on our experiments combined with recent simulations [2], an intercalation model, accounting for the different periodicities observed in the interface layer, was proposed. These findings provide new insights into the strain-driven stabilization of intercalated metal layers and highlight the potential of graphene as a versatile platform for engineering low-dimensional materials.

[1] Adv. Mater. Interfaces 12, no. 21: e00617 (2025); [2] Appl. Surf. Sci. 681, 161572 (2025).

HL 19.5 Tue 11:45 HSZ/0201

Strain engineering in graphene on Ru(0001) — Paula García-Mochales[1] and •Antonio J. Martínez-Galera[1,2,3] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

The ability to induce and characterize strain in the atomic lattice of 2D materials, localized within only a few nanometers around specific positions, is a major challenge for the development of straintronics. In this work, the interaction between Si nanoparticles and the surface of graphene/Ru(0001) is employed to induce local strain in the latter. The strain field has been mapped at the nanoscale by scanning tunneling microscopy (STM), using the moiré pattern intrinsic to graphene/Ru(0001) surfaces as a magnifying lens. The induced strain is found to be confined within only a few nanometers around each nanoparticle. To achieve more accurate control, strain engineering at the nanometer scale was successfully performed by manipulating nanoparticles through the STM tip. This approach to controlled strain could provide a key tool for exploring new physics arising by strain in 2D materials.

Reference:
P. García-Mochales and A. J. Martínez-Galera, Nano Lett. 25, 16097-16103 (2025).

HL 19.6 Tue 12:00 HSZ/0201

Subsurface carbon controls graphene growth on Ir(111) — •Smruti Ranjan Mohanty, Lothar Brendel, Marko Kriegel, Niels Ganser, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

The CVD growth of 2D materials is governed by a balance between adsorption, surface diffusion, and nucleation. For transition metal substrates, dissolution into the bulk acts as an additional parameter. By employing in-operando low-energy electron microscopy (LEEM) to monitor graphene growth on Ir(111), the effect of the growth temperature and the precursor pressure on the nucleation behavior is studied. The island nucleation density exhibits two distinct regimes, described as separate cases within Venables nucleation theory [1]. For a critical nucleus size i* = 5, low dosing pressures yield a low nucleation density that is governed by incomplete condensation with a scaling exponent of 2.5. At higher-dosing pressures, adsorptions at island edges dominate over the adatoms loss into the substrate, resulting in a higher nucleation density and a strongly reduced scaling exponent. Kinetic Monte Carlo simulations that incorporate bulk dissolution reveal both nucleation regimes and find a universal, temperature-independent scaling law. The results indicate a universal nucleation behavior for 2D materials with finite, non-negligible solubility in the supporting metal substrate.

[1] J A Venables et al 1984 Rep. Prog. Phys. 47 399

HL 19.7 Tue 12:15 HSZ/0201

Thermodynamics of heteroatom-doped graphene: Brute forcing the partition function — •Lukas Hörmann[1,2], Benedict Saunders[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, United Kingdom — [2]University of Vienna, Austria

The introduction of dopants into graphene can be used to tune material properties for specific applications, such as electronics, sensors, or catalysis. Achieving such tunability requires precise control over the composition and concentration of dopants within the lattice. This demands a fundamental understanding of the thermodynamics that govern the phase space of heteroatom superstructures in the two-dimensional graphene framework. We present a comprehensive approach to determining dopant structures that enables the near-exhaustive enumeration of all relevant heteroatom superstructures. The approach combines Density Functional Theory and machine learning to build a transferable energy model for dopant formation. Our method's efficient data handling and fast inference enable the evaluation of more than 150 million possible structures, allowing us to effectively brute force the partition function and derive all thermodynamic properties from it. We show the capabilities of our approach for free-standing graphene doped with nitrogen atoms, establishing a thermodynamic model to investigate how temperature affects the configuration space of doped graphene. Our analysis yields physical insights into defect interactions. We observe a characteristic peak in the heat capacity, indicating an order-to-disorder transition, and present a mechanistic understanding of how this peak arises.

HL 20: Poster I

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

HL 20.1 Tue 18:00 P1

Defect-Mediated Electronic Reconstruction in Li-TFSI-Passivated Layered InI Crystals — •Abdulsalam Aji Suleiman[1,2], Ali Karatutlu[1,3], and Aydan Yeltik[4] — [1]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, Sivas 58000, Türkiye — [2]Sivas Cumhuriyet University Nanophotonics Application and Research Center (CÜNAM), Sivas 58140, Türkiye — [3]Institute of Materials Science Nanotechnology, National Nanotechnology Research Center (UNAM), Bilkent University, Ankara 06800, Türkiye — [4]Department of Material Science and Nanotechnology Engineering, TOBB University of Economics and Technology, Ankara 06560, Türkiye

Layered indium iodide (InI) is a van-der-Waals semiconductor whose bandgap (1.6-2.8 eV) enables strong light-matter coupling but suffers from iodine-vacancy defects that limit stability. Surface passivation with lithium bis(trifluoromethanesulfonyl)imide (Li-TFSI) modifies near-surface electrostatics and bonding, improving optical and transport properties. Photoluminescence shows stronger emission and longer carrier lifetimes, consistent with reduced non-radiative recombination. Soft-X-ray absorption spectroscopy at the HESEB beamline probes F, N, O, C K-edges and I M4,5-edges, revealing how TFSI-ions coordination alters In-I bonding and orbital hybridization. These results link chemical passivation and defect energetics, outlining a route to stable halide-based optoelectronic devices.

HL 20.2 Tue 18:00 P1

Tensor network methods for electron-hole complex in nanoplatelets — •Bruno Hausmann and Marten Richter — Institut für Physik und Astronomie, Technische Universität Berlin, Germany

Nanoplatelets are colloidally grown, atomically thin, rectangular semiconductor nanostructures. Excitons in nanoplatelets are solutions of a four-dimensional Schrödinger equation. This is especially true as the structure is in between the weak and strong confinement regimes. Solving this equation is computationally expensive compared to the typical two-dimensional Wannier equation under weak confinement. Going beyond excitons to trions and biexcitons, the memory size of the discretized wavefunctions grows exponentially with the particle number. Tensor network methods have successfully been applied to solve high-dimensional eigenvalue problems. Here we adapt them to the eigenvalue equation for excitons and trions by decomposing the real-space wavefunctions into quantics tensor trains (QTT). Operators that transform the indices, e.g. shift operators in finite differences, become binary circuits, e.g. an addition network. We were able to compute ground and excited states together with their energies for platelet dimensions between strong and weak confinement with a resolution (up to 2048 grid points per dimension) infeasible to implement without tensor networks. For illustration, eigenenergies, oscillator strengths, and various wavefunction projections were calculated.

HL 20.3 Tue 18:00 P1

Markovian vs. Full Quantum-Kinetic Approach to Phonon-Assisted Incoherent Exciton Formation in Atomically Thin Semiconductors — •Leonard Schneider, Andreas Knorr, and Henry Mittenzwey — Nichtlineare Optik und Quantenelektronik, Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Excitonic coherence decay and incoherent exciton formation in atomically thin semiconductors such as monolayer transition metal dichalcogenides are strongly influenced by the coupling between charge carriers and lattice vibrations. Based on Heisenberg's equations of motion, we derive the microscopic dynamics of excitonic transitions and incoherent exciton occupations coupled via phonon-assisted processes. For a consistent quantum-kinetical approach, we go beyond the usual one-phonon processes and include up to two-phonon-assisted and phonon-population-assisted transitions, which corresponds to a truncation of the hierarchy problem within a fourth-order Born approximation. We numerically evaluate the full quantum kinetics for the dephasing- and incoherent-exciton-generation dynamics and compare it to the corresponding Markovian limit. The corresponding influence of memory effects and multi-phonon processes is discussed in detail.

HL 20.4 Tue 18:00 P1

Far- and near-field photoluminescence of interlayer excitons in MoS2/WS2 heterostructures — •Johannes Holters and Iris Niehues — Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Monolayers of transition-metal dichalcogenides show intense photoluminescence (PL) at room temperature due to their high exciton binding energies. Recently, heterostructures composed of two vertically stacked monolayers have gained significant attention because of the emergence of novel quantum phenomena within these materials. Of particular interest are interlayer excitons, where, in contrast to intralayer excitons, electron and hole reside in different layers of the heterostructure. Strain, nanobubbles, Moiré effects and other local inhomogeneities can localize the appearance of these interlayer excitons to several nanometer. Here we use a scattering-type scanning near-field microscope (s-SNOM) to investigate the photoluminescence (PL) of interlayer excitons in a MoS2/WS2 heterostructure with a spatial resolution below the diffraction limit. The obtained tip-enhanced PL (TEPL) images are compared to standard confocal microscopy images. Both intra- and interlayer excitons are visible in far- and near-field images. In the TEPL images an enhanced PL signal is observed in the form of arcs around nanobubbles. These features can be assigned to interference effects caused by the interaction of the far-field light with the tip. Additionally, it is found that the intensity of the interlayer exciton PL strongly depends on the polarization of the exciting laser as well as the distance between tip and sample in the TEPL setup.

HL 20.5 Tue 18:00 P1

Optical Properties of CrSBr/TMD heterostructures — •Nicole Engel[1], Luc Oswald[1], Sai Shradha[1], Lukas Krelle[1], Daria Markina[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

Monolayer transition metal dichalcogenides (TMDs) exhibit several fascinating properties. These characteristics can be further expanded by creating heterostructures with CrSBr. CrSBr is an antiferromagnetic semiconductor which exhibits promising magnetic interactions with monolayer TMDs. The magnetic order of CrSBr influences the optical properties of $MoSe_2$ and WSe_2, facilitating charge transfer processes [1,2]. This work investigates CrSBr/TMD heterostructures using low-temperature optical spectroscopy with applied magnetic fields to probe excitonic properties. Understanding the optical and valley properties of CrSBr/TMD heterostructures will be relevant for the development of spintronic and valleytronic devices and show a great potential for light harvesting and enhancement of emission from 2D-materials.

[1] C. Serati de Brito et. al., Nano Lett. 2023, 23, 11073-11081
[2] J. de Toledo et. al., Nano Lett. 2025, 25, 13212-13220

HL 20.6 Tue 18:00 P1

Optical Properties of Interlayer Excitons in Transition Metal Dichalcogenide Heterostructures — •Luc Frederik Oswald[1], Sai Shradha[1], Nicole Engel[1], Julian Führer[1], Md. Tarik Hossain[2], Lukas Krelle[1], Daria Markina[1], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Institute for Physical Chemistry, Friedrich Schiller University, Jena, Germany

Interlayer excitons (IXs) in van der Waals heterostructures arise from electrons and holes confined in different monolayers, forming long-lived quasi particles with strong spin-valley coupling. In $MoSe_2/WSe_2$ systems, type-II band alignment and conduction-band splitting give rise to multiple IX states whose optical signatures are highly sensitive to temperature, lattice vibrations, and magnetic fields. This work investigates the optical response of an hBN-encapsulated, $MoSe_2/WSe_2$ lateral-vertical heterostructure grown via chemical vapour deposition (CVD). A combination of temperature-dependent photoluminescence, excitation-spectroscopy approaches, and magneto-optical measurements is used to probe the formation, evolution, and valley properties of interlayer excitons in this hybrid geometry. Together, they reveal characteristic interlayer emission features, their excitation pathways, and signatures of spin-layer hybridization.

HL 20.7 Tue 18:00 P1

Study of irradiation-induced deep-level defects in transition metal dichalcogenides MX2 (M = Mo,W; X = S, Se) — •Andrii Bodnar, Łukasz Gelczuk, and Paweł Scharoch — Departament of Semiconductor Materials Engineering, Wroclaw University of Science and Technology, Wybrzeze Wyspianskiego 27, Wroclaw 50-370, Poland

This work presents comprehensive density functional theory (DFT) calculations investigating native point defects in pristine and alpha-particle-irradiated MX_2 materials, where M represents Mo or W and X represents S or Se. The calculations focused on identifying deep-level defects and their charge transition levels, with subsequent experimental validation through deep level transient spectroscopy (DLTS) measurements. The satisfactory agreement between state-of-the-art DFT-calculated defect levels and DLTS experiments confirmed the reliability of the computational methodology and enabled identification of the origins of experimentally observed defect levels.

The validated DFT approach employing the HSE06 hybrid functional, which accurately predicts band gaps and eliminates self-interaction errors present in other approaches, was applied to calculate charge transition levels of defects in bulk MX_2 that are experimentally challenging to measure directly using DLTS. Using DFT-generated data, deep-level defects induced by alpha-particle irradiation in bulk MX_2 were identified and defect evolution under different irradiation doses was tracked.

HL 20.8 Tue 18:00 P1

Influence of hBN encapsulation on the degradation process of Hittorf phosphorus — •Maximilian Scharpey[1], Daniel Wigger[2], Nicolas Pajusco[3], Iker Herrero[3], Rainer Hillenbrand[3], and Iris Niehues[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany — [3]CIC nanoGUNE BRTA, Donostia-San Sebastián, Spain

The van-der-Waals material Hittorf phosphorus (HP, violet phosphorus) has attracted increasing interest due to its promising semiconducting properties including high charge carrier mobility, a tuneable bandgap, and high optical absorption in the visible [1]. However, its degradation poses significant challenges for device applications. Here, we investigate the influence of hexagonal boron nitride encapsulation on the optical properties of thin flakes of mechanically exfoliated HP. By comparing photoluminescence and nanoscale Fourier transform infrared spectroscopy of encapsulated and non-encapsulated HP samples over a period of days, we gained insight on the degradation process. In addition, we used scattering-type scanning near field optical microscopy to localize the origin sites of degradation under the encapsulation layer with a resolution beyond the diffraction limit. These findings contribute to a deeper understanding of the degradation process of HP, which will play a crucial role in stabilizing this material for future applications.

[1] Ahmad et al., Adv. Funct. Mater. **34**, 2410723 (2024)

HL 20.9 Tue 18:00 P1

Graphene/WSe_2 heterostructures for optical investigation of proximity spin-orbit coupling — •Ernst Knöckl, Matthias Klein, Alexander Holleitner, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

We investigate proximity-induced spin-orbit coupling (SOC) in graphene/WSe_2 heterostructures using the circular photogalvanic effect (CPGE) as a symmetry-selective, experimentally simple optical probe of spin-valley-locked band textures [1]. By measuring helicity-dependent photocurrents as a function of gate voltage, excitation energy, and device geometry, we aim to disentangle Rashba and valley-Zeeman SOC contributions and to extract their magnitude and sign as a function of the graphene-WSe_2 twist angle. A key requirement is the fabrication of large, clean, and field-effect-gateable graphene/TMDC heterostructures. To this end, we demonstrate a modified dry-transfer process based on specifically prepaired polydimethylsiloxane (PDMS) stamps [2]. We further determine the relative twist angle using Raman spectroscopy and second-harmonic generation (SHG) spectroscopy.

[1] Kiemle, Jonas, et al. ACS nano 16.8, 12338-12344 (2022)
[2] Jain, A. et al. Nanotechnology 29.26, 265203 (2018)

HL 20.10 Tue 18:00 P1

Transport measurements in thin layers of $HfTe_5$ — •Freddy Sack[1], Christopher Belke[1], Sonja Locmelis[2], Lina Bockhorn[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität, 30167 Hannover, Germany

Hafnium pentatelluride ($HfTe_5$) gained interest due to its topological insulator behavior and the pronounced anisotropy arising from highly disparate electron and hole masses. In recent works, a thickness dependent band gap was observed [1]. In contrast to the small band gap found in bulk $HfTe_5$, single layers are predicted to be quantum spin hall insulator with a large band gap [1-4]. In this study, we investigate temperature dependent transport properties of thin layers of $HfTe_5$ from 5 K to 270 K. Gate dependent measurements for different magnetic fields are utilized to characterize thin flakes with a thickness less than 50 nm and to investigate the resistance anomaly.

[1] C. Belke et al., 2D Mater. 8, 0350292021 (2021)
[2] K.C Dogan et al., Nanoscale, 16, 11262 (2024)
[3] Ling-Xioa Zhao et al., Chinese Phys. Lett. 34 037102 (2017)
[4] Bo Fu et al., Phys. Rev. Lett. 125, 258801 (2020)

HL 20.11 Tue 18:00 P1

Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures Reveals Peak Splitting in 2D Polar Silver — •Ulrich Limberg[1], Jakob Henz[1], Siavash Rajabpour[2], Alexander Vera[2], Arpit Jain[2], Joshua A. Robinson[2], Su Ying Quek[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, Munster, Germany — [2]MatSE PennState, Pennsylvania, USA — [3]Centre of Advanced 2D Materials, Signapore, Signapore

Two-dimensional (2D) polar metals are a new class of atomically thin materials created by confinement heteroepitaxial growth, where metallic species such as silver are intercalated between epitaxial graphene and a 6H-SiC substrate [1]. Silver intercalation leads to two competing semiconducting monolayer phases, the metastable Ag(1) and the stable Ag(2), each showing distinct opto-electronic behaviour [2].

Spectroscopic imaging ellipsometry (SIE) enables spatially resolved analysis of the complex dielectric function of both phases. Using temperature-dependent SIE from 5 K to room temperature, we investigate the modification of the linear light-matter interaction of 2D polar Ag with temperature. At low temperatures, we detect a splitting of the characteristic absorption peak of Ag(2). The experimentally determined dielectric function agrees well with theoretical predictions [2].

[1] N. Briggs et al., Nat. Mater. 19.6, 637-643 (2020).
[2] A. Jain et al. in preparation (2025).

HL 20.12 Tue 18:00 P1

Structural and Electrical Characterization of Graphene Thin Films from Dispersions — •Yasaman Jarrahi Zadeh[1], Lars Grebener[2], Shaghayegh Pourdahrany[3], Muhammad Ali[4], Nicholas Wilson[5], Mohaned Hammad[2], Günther Prinz[1], Martin Geller[1], Michael A. Pope[5], William Wong[3], Hartmut Wiggers[4], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics, and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Energy and Materials Processes, and CENIDE, University of Duisburg-Essen, Germany — [3]Department of Electrical and Computer Engineering, and WIN, University of Waterloo, Canada — [4]Institute for Combustion and Gas Dynamics, and CENIDE, University of Duisburg-Essen, Germany — [5]Department of Chemical Engineering, and WIN, University of Waterloo, Canada

Graphene powders were produced by microwave-plasma synthesis and sonicated into ethanol or water with carboxymethyl cellulose (CMC) or di-n-dodecyl dimethylammonium bromide (DDDA) stabilizers. Using ultrasonic spray coating or Langmuir deposition, thin films were deposited on sapphire and characterized by SEM, Raman spectroscopy, and transport measurements. Water-based CMC dispersions produced the most uniform films. Raman spectra showed good structural quality (judged by the intensity ratio $I_{2D}/I_G \sim 1.5$). CMC-stabilized spray-coated films (0.1 wt%) achieved the highest conductivity (2.5 mS) and mobility (11 cm^2/V.s). DDDA films were more porous with lower mobility, while multilayer Langmuir films reached higher mobility (19 cm^2/V.s) but reduced conductivity.

HL 20.13 Tue 18:00 P1

Raman polarization switching in CrSBr — Priyanka Mondal[1], Daria Markina[1], •Lennard Hopf[1], Lukas Krelle[1], Sai Shradha[1], Julian Klein[2], Mikhail Glazov[3], Iann Gerber[4],

Kevin Hagmann[1], Regine v. Klitzing[1], Ksenija Mosina[5], Zdenek Sofer[5], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology — [3]St. Petersburg, Russia — [4]Université de Toulouse, INSA-CNRS-UPS, LPCNO — [5]Department of Inorganic Chemistry, University of Chemistry and Technology Prague

In recent years, few-dimensional nanomaterials have sparked significant interest within the solid-state research community due to their novel properties and possible applications in quantum technologies. Layered CrSBr has attracted particular interest due to its quasi 1D nature, strong electron-phonon interaction and air-stability. This work probes the optical anisotropy using polarization resolved photoluminescence and Raman spectroscopy on mono and few-layer CrSBr. These techniques are sensitive to the crystal orientation and reveal the intricate dependence of phonon polarization on excitation energy. Additionally, a clear thickness dependence of the electronic and vibrational properties is found. These results shed light on the complex electron-phonon and photon-phonon interactions in CrSBr opening new avenues for future application in optoelectronic devices.

HL 20.14 Tue 18:00 P1

Tuning carrier type and electrical properties of 2D alloy transistion metal dichalcogenides — •Axel Printschler, Md Tarik Hossain, Nhat Lam Duong, Julian Picker, Rahul Sharma, Christof Neumann, Muhammad Sufyan Ramzan, Caterina Cocchi, and Andrey Turchanin — Friedrich Schiller University Jena, Germany

Two-dimensional (2D) transition metal dichalcogenide (TMD) alloys offer a powerful platform for engineering material properties beyond the limitations of their constituents. Controlling the electronic characteristics of TMDs is crucial for the development of advanced electronic and optoelectronic devices and functional circuitry. This study focuses on the electronic properties of monolayer $(V_xW_yMo_{1-x-y})S_2$ alloys synthesized via a liquid-precursor-based chemical vapor deposition (CVD) approach. We investigate the charge transport in these materials using field-effect transistor (FET) devices. Our electrical measurements demonstrate a controlled transition from n-type to p-type semiconducting behavior, culminating in a metallic state for high vanadium concentrations. This change is supported by density functional theory (DFT) calculations. The tunability, directly correlated with the alloy composition, provides a reliable strategy for tailoring the electronic character of 2D TMDs and underscores their significant potential for application in next-generation electronic devices.

HL 20.15 Tue 18:00 P1

Many-body effects and intervalley coupling mechanisms in monolayer transition metal dichalcogenides — •Oleg Dogadov[1,2], Henry Mittenzwey[3], Thomas Deckert[4], Micol Bertolotti[2], Daniele Brida[4], Giulio Cerullo[2,5], Andreas Knorr[3], and Stefano Dal Conte[2] — [1]Fritz Haber Institute, Berlin, Germany — [2]Politecnico di Milano, Milan, Italy — [3]Technische Universität Berlin, Berlin, Germany — [4]University of Luxembourg, Luxembourg — [5]CNR-IFN Milan, Italy

The strongly bound excitons and the spin-valley locking effect make monolayer (1L) transition metal dichalcogenides (TMDs) an ideal platform to study intra- and intervalley many-body effects. Despite extensive studies conducted during the last years, a unified description of the competing many-body interactions and intervalley coupling processes in 1L-TMDs is lacking. Here, we apply broadband helicity-resolved transient absorption spectroscopy combined with a microscopic theory based on the excitonic Bloch equations to investigate coherent optical response and valley polarization dynamics in 1L-WSe_2. We unambiguously unravel competing valley-dependent contributions of two- and four-particle correlations to the coherent optical response of the studied material. By exploring the valley (de)polarization dynamics, we dissect the roles of individual intervalley coupling mechanisms, including Coulomb exchange and Dexter-like interaction, as well as phonon-assisted scattering, providing a consistent picture of the processes governing spin-valley dynamics in 1L-TMDs.

HL 20.16 Tue 18:00 P1

Unconventional Nanopatterning of 2D Materials for Future Nanoelectronics — •Tawat Chen[1,2], Poonam Borhade[3], Ya-Ping Hsieh[4], and Mario Hofmann[1] — [1]Department of Physics, National Taiwan University, Taipei, 10617 Taiwan — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 3, 07743 Jena, Germany — [3]Institute of Physics, Academia Sinica, Taipei, 10617 Taiwan — [4]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617 Taiwan

Two-dimensional (2D) materials offer a promising pathway to surpass the physical scaling limits of silicon-based electronics in the post-Moore era. However, fabricating high-resolution nanofeatures on these materials using conventional photolithography is constrained by Rayleigh's diffraction limit and escalating processing costs. In this work, we demonstrate nanopatterning techniques that overcome these limitations. First, we utilize a self-expansion double patterning (SEDP) process to generate nanometer-scale features through a self-limiting, temperature-controlled oxidation mechanism, enabling the fabrication of graphene nanoribbons with precise control. Second, to achieve high-density patterning without standard lithography, we investigate the formation of porous anodic aluminum oxide (AAO) via anodization, successfully creating porous arrays with a diameter of 37 nm. Finally, we discuss the physical mechanisms governing these formation processes and their potential for the scalable, high-throughput fabrication of next-generation 2D material devices.

HL 20.17 Tue 18:00 P1

Universality of Raman spectroscopy for determining twist angle in diverse systems — •Ana Senkić[1], Nicolai Leonid Bathen[2], Thorsten Deilmann[1], Hendrik Lambers[1], Lara Blinov[1], Aleksandar Matković[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Israel Institute of Technology, Haifa, Israel — [3]Chair of Physics, Department Physics, Mechanical Engineering, and Electrical Engineering, Montanuniversität Leoben, Leoben, Austria

Twisted bilayers of transition metal dichalcogenides form moiré superlattices, resulting in electronic moiré minibands [1]. Correlated phases hosted in these structures are prone to twist disorder given by lateral fluctuations of the moiré cell size [2]. We investigated this lateral twist inhomogeneity on twisted WSe2 bilayers using comprehensive correlative lateral force microscopy and Raman spectroscopy [3].

In this work, we expand the topic by investigating different twisted systems: artificially stacked fully encapsulated WSe2 bilayers, MoSe2/WSe2 hetero-bilayers and CVD-grown MoS2 bilayers. Moiré phonon frequencies obtained from Raman spectroscopy maps are utilized to determine the twist angle over micrometer-sized areas in these systems. Additionally, Raman mapping facilitates fast and non-destructive identification of homogeneous, high-quality regions in encapsulated and gated structures.

[1] N. Saigal, et. al., Phys. Rev. Lett. 133, 046902 (2024) [2] S. Shabani et al. Nat. Phys. 17, 720-725 (2021) [3] N.L. Bathen et al. in preparation

HL 20.18 Tue 18:00 P1

Nonlinear interference in a CrSBr BIC metasurface — •Fabian Glatz[1], Thomas Weber[2], Till Weickhardt[1], Luca Sortino[2], Andreas Tittl[2], and Giancarlo Soavi[1] — [1]Friedrich Schiller University Jena — [2]Ludwig Maximilians University of Munich

The active electrical [1] and all-optical [2] modulation of the nonlinear optical (NLO) response of layered materials has attracted great interest for nanophotonic applications. Ferroic layered materials, such as CrSBr, offer an alternative and powerful approach for NLO tuning thanks to temperature-dependent phase transitions [3]. Here, we present a new method where NLO modulation arises from interference effects between bound states in the continuum (BIC) resonances and the bulk NLO susceptibility of a CrSBr nanophotonic device. To achieve this, we patterned exfoliated CrSBr flakes into metasurfaces that exhibit BICs and investigated their NLO response. By varying the dimensions of the metasurface, we obtain direct control over the energy, linewidth and Q-factor of the BIC resonances [4]. When the energy of the BIC resonance is close to that of the CrSBr exciton, we further observe a strong modulation in third harmonic generation (THG), characterized by both constructive and destructive interference depending on the energy of the emitted TH signal. These results allow us to retrieve the real and imaginary parts of the BIC-resonance, and they further demonstrate a new powerful approach for NLO engineering at the nanoscale. *[1] Soavi et al. Nat. Nanotech. 13, (2018). [2] Klimmer et al. Nat. Photon. 15, (2021). [3] Wang et al. Nat. Com. 14, (2023). [4] Weber et al. Nat. Mater. 22, (2023).*

HL 20.19 Tue 18:00 P1

Surface acoustic wave spectroscopy on low dimensional semi-

conductor materials — •Paul Hollatz, Felix Ehring, Paromita Bhattacharjee, Emeline Nysten, and Hubert Krenner — Intitute of Physics, University of Münster, Germany

For future technologies, low-dimensional quantum materials such as 2D transition metal dichalcogenides (TMDCs), 1D Nanowires, or 0D Quantum Dots (QDs) are of highest relevance.

Studying the properties of such semiconductor nanomaterials can be achieved by various methods, including the combination of surface acoustic wave (SAW) spectroscopy and photoluminescence (PL) measurements, which provides unique access to carrier dynamics.

In this approach, SAWs operating in the MHz to GHz regime enable on-chip integration due to their micro- to nanometer wavelengths.

Here, we show that interaction of a SAW with co-integrated materials via its strain and the electrical field enables contact-free sensing and manipulation of their optical properties.

When combined with time-integrated and time-resolved PL measurements, it reveals excitation pathways and charge-carrier behaviour, offering deeper insight into the fundamental processes that govern these materials and paving the way for advanced optoelectronic applications.

HL 20.20 Tue 18:00 P1

Interfacial Electronic Coupling in WS2-PyMACl van der Waals Heterostructures — •Mohammed Adel Aly[1,2], Dominik Muth[3], Bettina Wagner[4], Martin Koch[2], Johanna Heine[4], and Marina Gerhard[3] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [2]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Semiconductor Photonics Group, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Semiconductor Spectroscopy Group, Philipps-Universität Marburg, 35032 Marburg — [4]Department of Chemistry and Marburg Centre for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany

Interfacial coupling in mixed van der Waals systems enables tuning of the optical response of 2D semiconductors. We investigate heterostructures based on monolayer WS2 and few-layer organic crystalline pyrenemethylammonium chloride (PyMACl). Time-resolved photoluminescence shows a pronounced shortening of the PyMACl emission lifetime, indicating efficient interfacial coupling. Polarization-resolved measurements show a clear polarization anisotropy in WS2 within the heterostructure, pointing to symmetry breaking induced by the organic crystal. These observations demonstrate electronic coupling across the interface and highlight ionic organic crystals as functional substrates for tailoring excitonic behavior in 2D materials.

HL 20.21 Tue 18:00 P1

Optical Properties of a Transition-metal Dichalcogenide - ZnO Nanowire Field-effect Transistor — •Yashvi Bulsara[1], Maximilian Tomoscheit[1], Omid Ghaebi[1], Edwin Eobaldt[1], Carsten Ronning[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, University of Jena — [2]Abbe Center of Photonics, University of Jena

Transition-metal dichalcogenide (TMD) monolayers combined with zinc-oxide (ZnO) nanowires (NW) represent a promising platform for electrically tunable nanophotonic devices. ZnO NWs can be used as nanoscale lasers, supporting waveguiding, field amplification and being the gain medium at the same time. A further major step towards the success and broad applicability of NW lasers, is the possibility to actively tune their laser properties via external stimuli, such as the piezo-electric effect[1]. Recently, we have demonstrated that coupling of ZnO NWs to monolayer TMDs leads to an increase of the lasing intensity threshold[2]. Building on this approach, in this poster I will propose a device where the laser emission of a ZnO NW can be electrically tuned by coupling it to a TMD based field-effect transistor. Besides the main idea and device architecture, I will present preliminary results of device fabrication and characterization.

[1] M. Zapf, Nano Lett., 2017, 17 (11), 6637-6643
[2] E. Eobaldt, Nanoscale, 2022,14, 6822-6829.

HL 20.22 Tue 18:00 P1

Optical Properties of He^+-Irradiated CrSBr — •Alison Pfister[1], Daria Markina[1], Shengqiang Zhou[2], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

CrSBr, a van der Waals layered magnet, exhibits rich interactions among quasiparticles, involving photons, excitons, and spins. Although antiferromagnetic in its bulk pristine form with ferromagnetic intralayer order, irradiation with He^+ ions drives CrSBr into a ferromagnetic state, enabling novel optical behaviour without applying an external magnetic field. We probe the optical response using polarization-resolved Raman spectroscopy together with absorption and photoluminescence excitation (PLE) measurements. Pronounced changes in Raman intensity and polarization alongside marked variations in absorption near the Curie temperature, and resonant features in PLE spectra were observed. Analysis of Raman tensor evolution and anomalous temperature-dependent behaviour of excitons in absorption highlights intricate coupling between lattice, electronic, and magnetic states, positioning CrSBr as an attractive platform for exploring quasiparticle physics in 2D magnets and related quantum technologies.

HL 20.23 Tue 18:00 P1

Creating Chalcogenide Aeromaterials through Atomic Layer Deposition — •Vladimir Ciobanu[1], Alejandra Ruiz-Clavijo[2], Tudor Braniste[1], Sebastian Lehmann[2], Niklas Wolff[3], Dongho Shin[2], Eduard Monaico[1], Rainer Adelung[3], Lorenz Kienle[3], Kornelius Nielsch[2], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany — [3]Kiel University, Kiel, Germany

In this work, we report the development of SnS2 and SnSe2 aeromaterials synthesized via ALD on sacrificial ZnO microtetrapod templates. The ALD process enables conformal coating of the 3D ZnO microtetrapod network with precise thickness control. The resulting SnS2 and SnSe2 shells retain the original tetrapodal morphology after selective ZnO removal in acid, forming a hollow microtubular structure with the wall thickness of about 50 nm and very high porosity. Structural characterization by XRD revealed that the as-deposited films are amorphous, while post-deposition annealing in a S or Se atmosphere at 250 °C induces crystallization of SnS2 or SnSe2. SEM demonstrated uniform coverage and preservation of the porous aeromaterial network. TEM revealed the presence of SnSx or SnSex phases with multidomain. These results highlight the capability of ALD to fabricate crystalline, compositionally controlled, and geometrically complex chalcogenide aeromaterials with strong potential for photoactive and catalytic applications. Acknowledgements: We thank the BMFTR and NARD for the funding of ProMoMo project DEHYCONA.

HL 20.24 Tue 18:00 P1

Creating Chalcogenide Aeromaterials through Atomic Layer Deposition — •Vladimir Ciobanu[1], Alejandra Ruiz-Clavijo[2], Tudor Braniste[1], Sebastian Lehmann[2], Niklas Wolff[3], Dongho Shin[2], Eduard Monaico[1], Rainer Adelung[3], Lorenz Kienle[3], Kornelius Nielsch[2], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany — [3]Kiel University, Kiel, Germany

In this work, we report the development of SnS2 and SnSe2 aeromaterials synthesized via ALD on sacrificial ZnO microtetrapod templates. The ALD process enables conformal coating of the 3D ZnO microtetrapod network with precise thickness control. The resulting SnS2 and SnSe2 shells retain the original tetrapodal morphology after selective ZnO removal in acid, forming a hollow microtubular structure with the wall thickness of about 50 nm and exceptionally high porosity. Structural characterization by XRD revealed that the as-deposited films are amorphous, while post-deposition annealing in a S or Se atmosphere at 250 °C induces crystallization of SnS2 or SnSe2. SEM demonstrated uniform coverage and preservation of the porous aeromaterial network. TEM revealed the presence of SnSx or SnSex phases with multidomain. These results highlight the capability of ALD to fabricate crystalline, compositionally controlled, and geometrically complex chalcogenide aeromaterials with strong potential for photoactive and catalytic applications. Acknowledgements: We thank the BMFTR and NARD for the funding of ProMoMo project DEHYCONA.

HL 20.25 Tue 18:00 P1

Investigating few-layer 3R-MoS_2 on top of laser-written waveguides — •Elisabeth Grune[1], Alina Schubert[1], Karoline Becker[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Takashi Taniguchi[3], Kenji Watanabe[3], Matthias Heinrich[1], and Tobias Korn[1] — [1]Insitute of Physics, University of Rostock, Rostock, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany — [3]National Institute for Material Science, Tsukuba, Japan

The properties of 3R-MoS_2, ranging from photoluminescence to second-harmonic generation, have attracted increasing scientific interest in recent years. Our goal is to couple these optical properties evanescently to an laser-written optical waveguide running along the substrate's surface. As a first step, we manufactured a system containing an hBN-encapsulated few-layer 3R-MoS_2 flake on top of a surface waveguide and investigated its photoluminescence signal in several optical geometries at room temperature as well as under cryogenic conditions. We find that when exciting the sample from above, the waveguide itself emits an unexpectedly high background fluorescence signal compared to the 3R-MoS_2 flake. We also use the waveguide itself to excite the flake, yet find that the previous fluorescence also dominates the spectrum. We discuss strategies for mitigating improving the present structures.

HL 20.26 Tue 18:00 P1

Transport simulations of bilayer graphene/WSe_2 electron-hole double quantum dots with spin-orbit coupling — •Nikita Berg[1,2], Hubert Dulisch[1,2], Roxana Anghel[1,2], Simone Sotgiu[1,2], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich

The electron-hole (e-h) symmetry in bilayer graphene (BLG) gives rise to robust spin-valley blockade in double quantum dots (DQDs) operated in the e-h regime. This enables the system to serve as a sensitive probe for blockade-breaking mechanisms. BLG/WSe_2 heterostructures offer electrostatic tunability of proximity-induced spin-orbit coupling (SOC) through the layer selectivity of the electron and hole wave functions in BLG. In this system, one possible spin-blockade-breaking mechanism arises from Rashba-type SOC, which can mediate spin-flip tunneling between the dots.

We present a master-equation-based steady-state transport simulation framework that accounts for coherence effects in e-h BLG double quantum dots. Using this approach, we show that Rashba-mediated spin-flip tunneling produces a distinctive dependence of the e-h blockade lifting on the angle of the applied in-plane magnetic field. This predicted angular dependence provides a clear and experimentally testable signature of induced Rashba spin-orbit coupling in BLG/WSe_2 heterostructures.

HL 20.27 Tue 18:00 P1

Active Fabri-Perot interferometer cavity stabilization for high-resolution spectroscopy of low-light single-photon emitters — •F. Stechemesser[1], F. Schaumburg[1], C. Dietrich[2], H. Mannel[1], A. Rodriguez[2], J. König[2], C. Steiner[3], P. Pesch[3], A. Lorke[1], G. Prinz[1], M. Geller[1], and A. Kurzmann[2] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany — [2]Physikalisches Institut Fachgruppe Physik, Universität zu Köln, Germany — [3]Fachgruppe Physik, RWTH Aachen, Germany

Single-photon emission from solid-state quantum emitters, such as quantum dots and defects in 2D materials, with narrow linewidths is one of the key ingredients for future applications in quantum information processing. In photoluminescence spectroscopy, the linewidths of such emitters can be determined using a grating spectrometer. However, in resonance fluorescence and at low laser excitation intensity, such spectrometers reach their limits regarding resolution and optical sensitivity. We introduce an actively stabilized, narrow-linewidth (free spectral range of 30 GHz) Fabry-Perot interferometer (FPI) that is stabilized using the light from a frequency-tunable diode laser. The quantum emitter photons are sent through the FPI, which is scanned across the emitter resonances. This approach enables measurements on a single photon detector (APD) with extended integration times. The single photon sensitivity of an APD can then be used to resolve low-intensity optical resonances of the different quantum emitters with a resolution down to 60 MHz. We show first results of single photon emission from InAs quantum dots and defects in WSe_2 monolayers.

HL 20.28 Tue 18:00 P1

Temperature-Dependent Studies of Interlayer Exciton in PbI2/WS2 Heterostructure — •Tobias Mantheі[1], Bhabani Sahoo[1], Ajay Kumar[2], Abhishek Misra[2], Chirag Palekar[1], and Stephan Reitzenstein[1] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India; Center for 2D Materials Research and Innovation, IIT Madras, Chennai 600036, India

We present temperature-dependent studies of interlayer exciton in PbI2/WS2 heterostructure. The interlayer exciton formed in such heterostructures consist of electron and hole situated at gamma point in Brillouin zone of respective materials. Hence these dipolar exction are twist angle independent and momentum direct while emitting at room temperature. Taking advantage of the stable nature of the interlayer exciton we investigated radiative lifetime along with polarisation as function of the temperature. We observe relatively long radiative lifetime at low temperature compared to room temperature. Furthermore, we measured the polarisation of the interlayer exciton, which suggests that the emission is elliptically polarised, with peak splitting occurring at high temperatures. This provides insight into spin-valley dynamics. Our studies establish solid foundation for further light-matter interaction experiments related to room temperature interlayer excitons integrated in microcavity.

HL 20.29 Tue 18:00 P1

Effective Theory of Feshbach Resonances in Two-Dimensional Semiconductors — •Maximilian Wolf and Richard Schmidt — Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany

Feshbach resonances in two-dimensional semiconductor bilayer systems have recently been demonstrated through experiments and first-principles calculations. Motivated by these findings, we introduce an effective model that captures the essential physics of these resonances. We show how the model parameters can be fixed directly from experimental data, enabling us to derive analytical scattering phase shifts and propagators in the few-body limit. With these results, observables at finite chemical potential can be computed using standard many-body techniques. As an example, we evaluate the exciton absorption spectrum in TMD materials and compare our predictions with experimental observations.

HL 20.30 Tue 18:00 P1

Manipulation of hybrid interlayer excitons in homobilayer MoS_2 — •Ankur Arora, Mathias Federolf, Atanu Patra, Subhamoy Sahoo, Monika Emmerling, Anuj Kumar Singh, Simon Betzold, and Sven Höfling — Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

Van der Waals (vdW) heterostructures of transition metal dichalcogenide materials provide a versatile platform for novel excitonic phenomena. Homobilayer MoS_2 is particularly attractive, as its hybrid interlayer excitons (hIX) possess a permanent dipole moment with high oscillator strength, even at room temperature and exhibit tunability via the quantum-confined Stark effect under an external DC electric field. In this work, we investigated the optical properties of hIX in homobilayer MoS_2, which is electrically contacted with few-layer graphene (FLG) and encapsulated in hexagonal boron nitride (hBN). The hBN encapsulation improves the optical response by narrowing the excitonic linewidths, revealing the effect of the dielectric environment. By applying a vertical electric field, we show the Stark splitting of the peaks of the hIX. The vdW heterostructure is transferred onto a distributed Bragg reflector (DBR) with pre-patterned contacts forming a half-cavity design. This architecture serves as a critical first step toward the fabrication of a full microcavity, enabling the exploration of strong light-matter coupling. Our results pave the way for electrically tuning these dipolar hIX polaritons inside a microcavity for fundamental studies on exciton condensates and exciton polariton-induced superconductivity.

HL 20.31 Tue 18:00 P1

SH modulation in a TMD-graphene heterostructure — •Raja Hoffmann[1], Lisa Suchomel[1], Omid Ghaebi[1], Till Weickhardt[1], and Giancarlo Soavi[1,2] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Abbe Center of Photonics, Jena, Germany

One of the most fascinating properties of layered materials is arguably the possibility to combine them in heterostructures with engineered electronic and optical properties. In the field of nonlinear optics, a clear example is the emergence of second harmonic generation (SHG)

in layered heterostructures realized by combining centrosymmetric materials. In such samples, interface broken space inversion symmetry can be engineered in different ways depending on the choice of materials and twist angle. An interesting example, which has been investigated recently in Ref.[1], are heterostructures composed of bilayer TMDs and monolayer graphene. As charges move from the TMD into the graphene, an imbalance between the bottom and top layers in the TMD bilayer leads to breaking of the inversion symmetry.
Building on these previous seminal results, we further investigate a bilayer TMD-monolayer graphene gated device, focusing in particular on both gate and all-optical tuneability of its engineered SHG. With this, we aim to add another prototype sample to the growing list of nonlinear nanophotonic devices based on layered materials and displaying ultrafast tunable optical properties [2,3].

[1] Zhang et al. Science Advances 9, 4571 (2023).
[2] Ghaebi et al. Advanced Science 11, 2401840 (2018).
[3] Klimmer et al. Nature Photonics 15, 837-842 (2021).

HL 20.32 Tue 18:00 P1

Electrical and optical studies of twisted graphene bilayers — •Anselm Watschke, Monica Kolek Martinez de Azagra, and Thomas Weitz — I. Physikalisches Institut, University of Goettingen

As a van der Waals heterostructure, twisted bilayer graphene shows rich angle-dependent electronic behavior, including magic-angle superconductivity [1] and near-30° interlayer decoupling [2], motivating efforts to tune its electrical properties through multiple degrees of freedom. Furthermore, in situ quantum twisting microscope measurements revealed the angle dependent tunneling current for small regions of twisted bilayer graphene [3].

In this work, we fabricated devices incorporating a locally twisted bilayer graphene region, enabling simultaneous investigation of the off-angle regime and adjacent monolayer domains. Encapsulation in hexagonal boron nitride was used to maintain the intrinsic behavior of graphene, and vibrational and electronic properties were subsequently examined through Raman spectroscopy and gate-tunable transport measurements.

[1] Cao, Y., Fatemi, V., Fang, S. et al. Nature 556, 43*50 (2018). https://doi.org/10.1038/nature26160
[2] H. Schmidt, T. Lüdtke, P. Barthold, E. McCann, V. I. Fal'ko, R. J. Haug; Appl. Phys. Lett. 27 October 2008; 93 (17): 172108. https://doi.org/10.1063/1.3012369
[3] Inbar, A., Birkbeck, J., Xiao, J. et al. Nature 614, 682*687 (2023). https://doi.org/10.1038/s41586-022-05685-y

HL 20.33 Tue 18:00 P1

Laser induced oxidation of thin layered MoS2 — •Aniketa Anampally, Gerhard Berth, Klaus Jöns, and Henry Hübschmann — Paderborn University, Germany

Transition metal dichalcogenides (TMDs) have gained great attention within the growing field of 2D materials. Due to their inherent semiconductor properties, materials like molybdenum disulfide (MoS2) have been implemented in many components of photonic and optoelectronic devices [1,2]. Precise structural modification has been proven to exhibit significant benefits to build tailored devices on the nanoscale [3]. In this work nonlinear microscopy is utilized for in-situ probing and laser oxidation of mechanically exfoliated 2H-MoS2. Precise locally resolved oxidation has been performed by second harmonic microscopy. The arising layer number dependency of this treatment is investigated further supported by polarization resolved analysis.

HL 20.34 Tue 18:00 P1

Optimization of quantum dot in nanowire for efficient emission in telecom spectral range — •Tomasz Gzyl[1], Giada Bucci[2], Valentina Zannier[2], Paweł Mrowiński[1], Anna Musiał[1], Elisa García-Tabarés[3], Ileana Florea[4], Beatriz Galiana[3], Lucia Sorba[2], Wojciech Rudno-Rudziński[1], and Grzegorz Sek[1] — [1]Wrocław University of Science and Technology, 50-370 Wrocław, Poland — [2]NEST Istituto Nanoscienze CNR and Scuola Normale Superiore, 56127 Pisa, Italy — [3]Universidad Carlos III de Madrid, 28903 Getafe, Spain — [4]CNRS-CHREA, 06560 Valbonne, France

One of the promising platforms for realization of a single photon source emitting in telecom wavelengths is an InAs(P) quantum dot (QD) embedded in a nanowire (NW), designed to enhance extraction efficiency and directionality of QD emission. Chemical Beam Epitaxy technique is employed to grow the QD within novel zinc-blende InP NW or wurzite InAsP NW. Here, we present numerical simulations of the QD-NW system, using finite-difference time-domain method to find optimal NW geometry for maximal extraction efficiency, within numerical aperture of 0.4 used in experiment and taking into account parameters space limited by the growth technology. To verify the calculations and further guide the growth of optimized structures, we performed micro-photoluminescence measurements as a function of excitation power on samples with different composition and NW shell diameter. The structural quality of the samples was confirmed using Scanning Transmission Electron Microscopy with Energy Dispersive X-ray Spectroscopy.

HL 20.35 Tue 18:00 P1

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

In this study, transient capacitance spectroscopy is used to examine the coupling between self-assembled quantum dots (SAQDs) - made of InAs in a GaAs heterostructure - in spatially separated layers. A rate equation model was developed, incorporating self-consistent band bending calculations, to describe the impact of the inter-layer coupling on the charge transfer processes. Here, also effects caused by the wetting layer are described and included into the model. The findings indicate that the coupling arises from the electrostatic field generated by the charged quantum dots in the adjacent layer as well as charge in a wetting layer, providing a quantitative explanation for the altered electron capture and emission dynamics.

HL 20.36 Tue 18:00 P1

Illumination Response of Electron Capture and Emission Dynamics in Self-Assembled Quantum Dots — •Till Draxler[1], Jan Lange[1], Julia Avdeev[1], Sven Scholz[2], Arne Ludwig[2], Andreas Wieck[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich-Heine University Düsseldorf — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

InAs Self Assembled Quantum Dots (SAQDs) are nanoscale semiconductor structures that confine charge carriers in all three spatial dimensions, leading to discrete, atom-like energy levels. Using Deep Level Transient Spectroscopy (DLTS) the influence of infrared irradiation with photon energies in respect to the bandgap energies of GaAs and InAs on the electron transfer dynamics is studied. To maintain a proper illumination of the SAQDs, semi-transparent NiCr Schottky gates are manufactured instead of classical Au gate.

HL 20.37 Tue 18:00 P1

Optimized quantum dot emitters for telecom applications: from growth to diode integration — •Tobias Bruggesser, Ponraj Vijayan, Patrick Pietrantuono, Sergej Vollmer, Philipp Noack, Justus A. Unfried, Ulrich Pfister, Michelle Weiss, Simone L. Portalupi, Michael Jetter und Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Germany

Quantum communication and quantum computing applications require a reliable high-purity single photon source. Stranski-Krastanov grown indium arsenide (InAs) quantum dots (QDs) are among the most widely studied candidates, as they possess high purity, brightness, and indistinguishability. When embedded in a GaAs semiconductor matrix, these QDs emit in the near-infrared region ($\approx$ 900 nm), and this can be shifted to the technologically important telecom C-band (1530-1565 nm) by introducing an InGaAs metamorphic buffer (MMB) beneath the QDs to engineer the strain. Our group has previously developed a thin InGaAs MMB based on a non-linear grading of the indium content with a so-called jump-convex-inverse (jci) design. This design is compatible with optical device fabrication, as it can be incorporated into a high-quality 1λ-cavity structure. In this work, we present our approach towards integrating these telecom C-band emitting InAs QDs into a p-i-n diode structure. Our goal is to control the charge carrier environment of the QDs, improve their optical properties, and achieve fine-tuning of the emission energy via the quantum-confined Stark effect.

HL 20.38 Tue 18:00 P1

Design and optimization of photonic nanostructures for

embedding GaAs quantum dots emitting at 780 nm — •Mrunmayee Deodhar[1], Ponraj Vijayan[1], Katharina Dahler[1], Ulrich Pfister[1], Michelle Weiss[1], Melina Peter[2], Ailton José Garcia Jr.[2], Thomas Oberleitner[2], Michael Jetter[1], Simone Luca 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 for single and highly indistinguishable photons. Their optical properties like a narrow wavelength distribution, short decay times, linewidths close to the Fourier limit, and the resulting highly indistinguishable photons make them highly appealing for several quantum technologies. We demonstrate the integration of these QDs into photonic nanostructures such as single-mode waveguides, multimode interference splitters, and Bragg grating waveguides. We also present simulations and describe the fabrication process used to realize these photonic nanostructures.

HL 20.39 Tue 18:00 P1

Auger-recombination in no-wetting layer InAs self-assembled quantum dots — •M. Rasulyar[1], H. Mannel[1], F. Rimek[1], A. Ludwig[2], A. Lorke[1], and M. Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

The Auger-Meitner effect is a non-radiative recombination pathway in which the energy of an electron-hole pair is transferred to a third carrier. In colloidal quantum dots, this mechanism is known to suppress radiative emission, while in self-assembled InAs/GaAs quantum dots, both non-radiative Auger processes [1] and radiative Auger-like channels [2] have been reported. However, as Auger recombination is a dephasing effect in quantum dot-based single-photon devices, we study the influence of the confining potential on the non-radiative Auger recombination rate.

We investigate the Auger-Meitner dynamics in a no-wetting layer quantum dot incorporated in a gate-tunable p-i-n diode. Under resonant excitation of the trion transition, we observe a pronounced quenching of the resonance-fluorescence signal. The intensity reduction is quantitatively explained by the competition between the electron emission rate and the electron tunneling-in rate. The Auger recombination rate is in the order of $1\,\mu s^{-1}$ and in accordance with previous measurements with a rate of $\gamma_a = 2.3\,\mu s^{-1}$ [1]. [1]A. Kurzmann et al., Nano Lett. 16, 3367 (2016). [2]M. Löbl et al., Nat. Nanotechnol. 15, 558-562 (2020). [3]M. Löbl et al., Commun. Phys. 2, 93 (2019).

HL 20.40 Tue 18:00 P1

Single-electron charging events on double quantum dots in InSb nanowires — •Kanji Furuta[1], Marcus Liebmann[1], Fenja Thomsen[1], Sasa Gazibegovic[2], Diana Car[2], Erik Bakkers[2], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Dept. of Appl. Phys., Eindhoven Univ., The Netherlands

As a step to develop a single-electron counting tip for a scanning tunneling microscope, we investigate the charge states of a double quantum dot (DQD) formed in an InSb nanowire by monitoring the current through a floating-gate-coupled sensor quantum dot (QD). The DQD and sensor QD are defined electrostatically by bottom finger gates below hexagonal boron nitride (h-BN) used as the gate dielectric. Time-resolved measurements of the sensor QD current reveal single-electron charging events in the DQD. The asymmetric capacitive coupling of the floating gate allows us to identify which dot acquires an electron. The time traces of the double quantum dot movement of individual electrons are analyzed using full counting statistics, from which the Fano factor and factorial cumulants [1] are extracted.

[1] P. Stegmann *et al.*, Phys. Rev. B **92**, 155413 (2015).

HL 20.41 Tue 18:00 P1

Towards a Quantitative Framework for Capacitance-Voltage Spectroscopy in Quantum Dot Ensembles — •Phil Julien Badura[1], Nico Frédéric Brosda[1], Ismail Bölükbaşı[1], Ibrahim Engin[1], Patrick Lindner[1], Sascha René Valentin[1], Andreas Dirk Wieck[1], Björn Sothmann[2], and Arne Ludwig[1] — [1]Fakultät für Physik und Astronomie, Experimentalphysik VI, Ruhr-Universität Bochum, Bochum, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47048 Duisburg, Germany

This study investigates an inhomogeneous ensemble of quantum dots coupled to a charge reservoir using capacitance-voltage spectroscopy. Experimental measurements reveal shifts in capacitance peak positions influenced by AC frequency and temperature, with frequency-dependent shifts remaining unexplained by existing models. To address this, we develop a master-equation-based theoretical model incorporating energy-dependent tunneling effects, which successfully reproduces the experimental data. Our findings emphasize the role of energy-dependent tunneling in distinct regimes: at low temperatures, energy-level dispersion dominates, while at high temperatures and frequencies, shifts arise from optimized sequences of in- and out-tunneling events.

HL 20.42 Tue 18:00 P1

Towards the integration of telecom C-band QDs into photonic integrated circuits — •Michelle Weiss, Ulrich Pfister, Ponraj Vijayan, Simon Oberle, Justus Unfried, Philipp Noack, Tobias Bruggesser, Sergej Vollmer, Raphael Joos, Michael Jetter, Simone L. Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), University of Stuttgart, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, Germany

Photonic integrated circuits (PICs) pave the way to the realization of several quantum technologies on a small footprint, which makes them highly desirable for applications in quantum communication, computing, simulation and sensing. Silicon and silicon nitride are leading materials for PICs due to the high quality optical components and low optical propagation losses. Due to the indirect bandgap of silicon most of the single-photon sources (SPSs) are based on probabilistic implementations. However, the probabilistic generation of the photons can limit the scalability and requires the use of high laser powers, which is a potential drawback regarding the integration of on-chip detectors. In this regard, In(Ga)As quantum dots (QDs) are promising candidates as on-demand SPSs with high single-photon purity. For their integration on low-loss PICs, several approaches already exist, like monolithic integration techniques and hybrid approaches used for interfacing with silicon-based platforms. We present the progress on various PIC integration techniques for InGaAs QDs grown on a metamorphic buffer layer and so emitting in the telecom C-band.

HL 20.43 Tue 18:00 P1

Aharonov-Bohm interferometry with interacting quantum dots — •Oliver Oing, Alexander Hahn, Jürgen König, and Fred Hucht — Theoretische Physik, Universität Duisburg-Essen

We describe an Aharonov-Bohm interferometer consisting of two leads and two tunnel-coupled quantum dots with on-site Coulomb interaction using first order perturbation theory in the tunnelling strength. In earlier work, a diagrammatic approach was chosen. The complexity of the diagrams for arbitrary parameters limited the calculations to symmetric systems in energies and couplings. By developing a systematic routine in *Mathematica* to generate all possible diagrams, we can explore a wider range of system configurations. Eleven system parameters can be arbitrarily tuned, namely the finite Coulomb interactions, the quantum dot level energies as well as the tunneling strengths, magnetic flux, bias voltage and temperature, enabling us to describe both symmetric and asymmetric systems. A finite bias voltage makes it possible to explore the non-linear response regime. The routine calculates density matrix elements and uses these to obtain the occupations of the quantum dots, the current and the conductance through the system. With this, we compare to analytic results and numerically exact results obtained with the TraSPI method [1].

[1] S. Mundinar, A. Hahn, J. König, A. Hucht, Phys. Rev. B **106**, 165427 (2022)

HL 20.44 Tue 18:00 P1

Characterization of Quantum Dots after Rapid Thermal Annealing in Photonic Layer Structures — •Jasper Ullrich, Severin Krüger, Elias Kersting, and Arne Ludwig — Universitätsstraße 150, Bochum 44801

Rapid thermal annealing (RTA) is an effective post-growth technique for engineering the structural and optoelectronic properties of InGaAs quantum dots (QDs). Short, high-temperature pulses induce controlled interdiffusion that blueshifts the emission wavelength, reduces inhomogeneous broadening, and modifies carrier confinement. In this

work, we investigate how specific annealing conditions*temperature, duration, and ambient environment*govern these changes and, in particular, how they influence the oscillator strength of confined excitonic transitions. We expect to show that optimized RTA parameters significantly enhance radiative coupling of QDs, leading to increased oscillator strength and faster emission dynamics. These results would provide a systematic framework for tailoring the optical performance of InGaAs QDs for quantum-light sources, high-speed emitters, and infrared photonic devices.

HL 20.45 Tue 18:00 P1

Ohmic contact for charge tuning devices — •Krupali Dobariya[1], Tom Fandrich[1], Yiteng Zhang[1], Arijit Chakraborty[1], Sulabh Shrestha[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany. — [2]Leibniz Universität Hannover Laboratorium für Nano- und Quantenengineering, Schneiderberg 39, 30167 Hannover, Germany.

Semiconductor quantum dots have shown unique properties as deterministic single photon and entangled photon pair sources. Their outstanding optical properties have the potential for use in quantum applications like quantum communication, quantum key distribution and quantum computing. Nevertheless, due to the stochastic nature of the self-assembly growth process, quantum dots typically emit photons with a broad wavelength distribution across the entire chip, posing challenges for applications requiring specific wavelengths. To address this issue, various tuning techniques have been developed. Electrical tuning, in particular, has emerged as an effective method for adjusting the wavelength and mitigating charge noise in semiconductor quantum dots. Here we study the impact of contact fabrication on the emission properties of GaAs quantum dots. We aim to optimize the process of forming ohmic contacts to n- and p-doped GaAs, placing special emphasis on the selection of materials and the reduction of contact resistance. The quality and performance of the electrical contacts are evaluated through the photoluminescence characterization.

HL 20.46 Tue 18:00 P1

Mixed-dimensional Silicon Junctionless Nanowire Transistors with Hexagonal Boron Nitride Gate Dielectrics — •Ahmed Elwakeel[1,2], Sayantan Ghosh[1,2], Alessandro Puddu[1,2], Madhuri Chennur[1,2], Slawomir Prucnal[1], Yordan Georgiev[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]1Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany

The investigation of two-dimensional hexagonal boron nitride (hBN) as a gate dielectric arises from the intrinsic limitations of conventional oxide layers in aggressively scaled devices. Owing to its atomically thin structure, excellent insulating characteristics, and inherently clean surface free of dangling bonds, hBN enables improved electrostatic control and effective channel passivation. In Junctionless Nanowire Transistors (JNTs), which remain strong contenders for extending Moore's Law, the use of hBN offers the potential to suppress interface trap states and enhance carrier transport. In this work, a top-down fabrication approach was employed to define the n-type doped silicon nanowires (C = 1E19 cm-3). Two distinct JNT devices were prepared: one with native oxide and another incorporating a thermally grown oxide. Subsequently, exfoliated hBN flakes were dry-transferred onto both samples as a gate dielectric. The hBN-integrated JNTs with thermally grown oxide exhibited pronounced improvements in subthreshold swing, on-state current, and the ION/IOFF ratio.

HL 20.47 Tue 18:00 P1

Importance of Aluminium Quality for High-Quality Quantum Emitter — •Severin Krüger[1,2], Elias Kersting[1], Phil Badura[1], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Sparrow Quantum Aps, Copenhagen, Denmark

InAs quantum dots are regarded as excellent candidates for single photon emitters due to their high photon rates, good single photon properties, and compatibility with scalable and integratable photonic platforms.

Despite remarkable progress for quantum dots emitting at 950 nm, achieving the same results for quantum dots emitting in the important optical fibre transparency window around 1.3 *m has remained a major challenge.

Here we present a routine we used to monitor and improve the quality of aluminium containing layers grown in our MBE. We find that high quality Al in MBE significantly improves the interface quality and smoothness of Al(Ga)As layers by reducting the surface roughness.

These improvements enabled the growth of pristine distributed Bragg reflectors beneath a defect free, charge tunable quantum dot device, emitting near transform-limited single photons in the O-band at 1.3 um.

HL 20.48 Tue 18:00 P1

RoHS-Compliant Nanocrystal LEDs for Flexible Near-Infrared Biomedical Emitters — •Simon Letzer[1], Andrey Iodchik[2], Rabiul Islam[1], Vladimir Lesnyak[2], and Caroline Murawski[1] — [1]Institute of Solid State Electronics, TU Dresden, Germany — [2]Physical Chemistry, TU Dresden, Germany

The near-infrared (NIR) biological window enables deep-tissue access for non-invasive imaging and health monitoring. Wearable emitters for this range require flexible and efficient materials, yet organic LEDs lose performance above 850 nm. Colloidal nanocrystals (NCs) offer a promising alternative for NIR emission, although most efficient systems contain Hg, Cd, or Pb, restricting their use in biomedical settings. We therefore investigate RoHS-compliant NCs for solution-processed NIR emitters. As a baseline, we employed CdHgSe/CdZnS core/shell NCs, which have already demonstrated strong performance in LEDs and provide a reliable platform for optimizing device processing [1]. Film quality is strongly influenced by concentration, solvent, dispense time, spin profile, and baking conditions. High-boiling-point solvents produced uniform macroscopic films, while low-temperature baking and high spin speeds improved nanoscale smoothness. Building on these conditions, we fabricated our first RoHS-compliant devices based on CuInS2/ZnS NCs. Processing parameters were refined for this material, and different transport layers and device architectures were evaluated. These results demonstrate a viable path toward cadmium-free NIR emitters for wearable biomedical sensors.

[1] Adv. Funct. Mater. 2024, 34, 2310067.

HL 20.49 Tue 18:00 P1

Stark Tuning of CsPbBr3 Quantum Dots — •Christopher Borchers[1], Johann Dzeik[1], Maximilian Heller[1], Frederik Benthin[1], Eddy Rugeramigabo[1], Chenglian Zhu[2,3], Ihor Cherniukh[2,3], Gabriele Rainò[2,3], Maksym Kovalenko[2,3], Michael Zopf[1,4], and Fei Ding[1,4] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics, Empa - Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf — [4]Laboratory of Nano and Quantum Engineering, Leibniz University Hannover, Schneiderberg 39, D-30167 Hannover, Germany

CsPbBr3 perovskite quantum dots are bright, solution-processable nanocrystal emitters with size-tunable color and high oscillator strength. Furthermore, they can be fabricated and processed in a cheap and facile way. We investigate electric-field tuning of single dots through the quantum-confined Stark effect to minimize exciton fine-structure splitting and tune separate emitters into resonance with each other. This opens up possibilities of creating entangled photon pairs of super- and subradiance with perovskite quantum dot based photonic devices.

HL 20.50 Tue 18:00 P1

Low temperature dry etching of InAlAs/InP nanostructures for telecom band single photon sources — •Ankita Choudhary[1], Chenxi Ma[1], Yiteng Zhang[1], Eddy Patrik Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Epitaxial InP-based quantum dots are excellent candidates for telecom band single photon sources for long-distance quantum communication. Enhancing photon extraction requires integration into photonic nanostructures through high resolution lithography and dry etching. Conventional chlorine-based ICP-RIE etching of InP is challenging due to competing thermal demands that lead to uncontrollable volatilisation of chlorine byproducts at high temperatures, while low-temperature cyclic methods result in defect-rich interfacial layers.Here we demonstrate low temperature chlorine based etching that circumvents byproduct volatilisation and stoichiometric imbalance and elimi-

nates defect layer formation without intermediate chemical treatments. we demonstrate the fabrication of a submicron truncated cone with smooth sidewalls, enhancing spontaneous emission directionality. The fabricated nanostructure shows 3-4 times improved extraction efficiencies compared to as-grown samples, with an NA of 0.7 detection optics. This process provides a robust pathway for fabricating high-quality photonic nanostructures for quantum telecommunications.

HL 20.51 Tue 18:00 P1

Lateral Electric Field Tuning of Quantum Dots — •Johann Dzeik[1], Christopher Borchers[1], Chenxi Ma[1], Ankita Choudhary[1], Xian Zheng[1], Yiteng Zhang[1], Tom Fandrich[1], Arijit Chakraborty[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167, Hannover, Germany

Quantum dots are among the most promising material systems for single photon sources in quantum communication and computation. However, they exhibit a stochastic distribution of emission wavelengths and fine-structure splitting, necessitating post-growth tuning that must be compatible with their fabrication and photonic environment. In this study, we use planar electrodes in parallel and quadrupolar configurations at varying distances to investigate the influence of electric fields on the emission wavelength and fine-structure splitting of GaAs/ AlGaAs quantum dots.

HL 20.52 Tue 18:00 P1

SUPER Scheme in Telecom-Wavelength Quantum Dots — •Zenghui Jiang — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover

Co-authors: Vikas Remesh, Frederik Benthin,Thomas Bracht, Michael Jetter, Simone Portalupi, Doris Reiter, Peter Michler, Michael Zopf, Fei Ding

Abstract:

To obtain the best photon properties from quantum dots (QDs), direct driving between the S-shell and the ground state i.e., resonant excitation is typically required. However, laser filtering under resonant excitation is extremely challenging because the QD emission and the excitation laser lie at essentially the same wavelength. The recently proposed and experimentally demonstrated SUPER scheme addresses this challenge by using two relatively detuned laser pulses to directly drive the two-level system. Since the excitation and emission wavelengths are well separated, the scattered excitation laser can be spectrally filtered much more easily. In our work, we implement a pulse shaper based on a spatial light modulator to generate two well-defined laser pulses from a single broadband pulse for the SUPER scheme. In addition, we investigate SUPER excitation using two narrow-linewidth continuous-wave lasers as a comparison, enabling a clearer understanding of the excitation dynamics and the differences relative to pulsed operation.

HL 20.53 Tue 18:00 P1

Andreev Spin Qubits in Hole-Gas Based Nanowires with Mixed Superconducting Pairing — •Markus Plautz — Norwegian University of Science and Technology, Norway

Ge-based lower-dimensional hole gases proximitized by superconductors represent a promising platform for future quantum technologies, largely related to the complicated p-wave nature of the orbital wavefunctions of the valence band. While standard models often treat the induced superconductivity as purely s-wave, recent microscopic theories indicate that the proximity effect in these systems is far more complex. They reveal that the strong spin-orbit interaction can induce non-trivial mixed pairing correlations, featuring coexisting s- and p-wave terms.

We calculate the Andreev reflection phases and determine the Andreev bound state (ABS) energy spectrum in the presence of Zeeman and spin-orbit fields. In particular, we show how these odd-parity correlations influence the spin splitting, leading to distinct changes in the qubit energy levels. Furthermore, we discuss the coherent control of the qubit subspace by considering a time-dependent perturbation of the spin-orbit coupling. By deriving the exact transition matrix elements, we construct an effective Hamiltonian for the ASQ and investigate how this mechanism can be utilized to coherently drive the qubit.

HL 20.54 Tue 18:00 P1

Nonequilibrium transport in designed random obstacle arrays — •Frederik Bartels[1], Johannes Strobel[1], Beate Horn-Cosfeld[1], Mihai Cerchez[1], Klaus Pierz[2], Hans Werner Schumacher[2], Dominique Mailly[3], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany — [3]CNRS, Université Paris-Saclay, C2N Marcoussis, 91460 Marcoussis, France

Nonequilibrium transport phenomena in two-dimensional electron systems include Hall field induced resistance oscillations (HIROs), zero resistance states (ZRS), phase inversion of SdH oscillations, and modifications of the giant negative magnetoresistance (GNMR). In our recent work [1], we studied HIROs in two-dimensional electron gases dominated by scattering at artificially introduced, randomly distributed circular obstacles. For sufficiently high obstacle densities, these scatterers dominate the HIROs. The HIRO period increases with obstacle density, indicating a localization of the Hall field around the obstacles and providing an alternative explanation of the scaling factor γ in terms of spatially varying Hall fields. Here, we extend these studies to cross-shaped obstacle geometries designed to enhance backscattering - the central mechanism in the theory of HIROs [2]. The findings may help to establish a more unified understanding of nonlinear resistance oscillations in two-dimensional systems with artificial scatterers. [1] Bartels *et al.* Phys. Rev. B **111**, 165301 (2025), [2] Yang *et al.* Phys. Rev. Lett. **89**, 076801 (2002)

HL 20.55 Tue 18:00 P1

Tenfold Conductance Enhancement in Graphene Nanoscrolls via Interlayer Hopping — •Jia-Cheng Li[1], Yu-An Cheng[2], Ying-Je Lee[2], Xuan-Fu Huang[2], Yu-Jie Zhong[2], Carmine Ortix[3], and Ching-Hao Chang[2] — [1]Program on Key Materials, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 70101, Taiwan — [2]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Rolling a graphene nanoribbon into a nanoscroll, a radial superlattice, offers a simple yet powerful way to control electronic transport at the nanoscale. In this work, we show that a one-turn nanoscroll exhibits a dramatic enhancement of quantum conductance compared to a flat ribbon, reaching nearly an order of magnitude in our tight-binding transport calculations. This effect does not rely on curvature-induced gauge fields or external perturbations. Instead, it arises purely from interlayer hopping at the overlapping edges of the scroll, which hybridizes the zigzag edge states and reconstructs the low-energy band structure. The resulting collapse of the flat bands reduces the density of states and shifts the Fermi level upward at fixed carrier density, activating multiple propagating modes. As the number of turns increases, these effects gradually weaken. Our findings identify nanoscrolls as a tunable geometry-driven platform for engineering transport in low-dimensional carbon systems.

HL 20.56 Tue 18:00 P1

Top-Down Fabrication and characterization of Al-Si-Al Nanowire Schottky barrier field-effect transistors — •Banafsheh Aghvami[1], Alessandro Puddu[1,2], Ahmed Elwakeel[1,2], Sayantan Ghosh[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01069, Germany

In Schottky barrier field-effect transistors (SBFETs), the channel length plays a crucial role in device performance. Shorter channels lead to lower channel resistance, stronger electrostatic gate control, reduced threshold voltage, and improved ON/OFF current ratios. However, to achieve sub-100 nm channel lengths using conventional top-down patterning approaches is extremely challenging due to resolution limits, line-edge roughness, and probable alignment errors. In contrast, the Al-Si-Al solid-state exchange process via rapid thermal annealing (RTA) enables the formation of well-defined and self-aligned short silicon channels. In this study, electron beam lithography (EBL) is used to define nanowire structures into HSQ resist. Then, the patterned structures will be transfered into the silicon layer by Inductively Coupled Plasma-Reactive Ion Etching (ICP-RIE). The Aluminium metal contacts will be formed by sputtering deposition. Scanning Electron Microscopy (SEM) will be employed to analyse the Al-Si-Al heterostructure. In addition, the performance of fabricated SBFETs will be evaluated by electrical characterisation using back-gated configuration.

HL 20.57 Tue 18:00 P1

Organic LEDs for optogenetic cochlear implants — •Nirbhika Nandakumar and Caroline Murawski — Dresden University of Technology, Dresden, Germany

Recent studies have highlighted the potential of optogenetic cochlear implants (oCIs) to surpass the spatial resolution limitations of conventional electrical stimulation by utilizing confined light to activate genetically modified auditory neurons [1]. Existing oCI prototypes predominantly use micro-LEDs, which can generate high optical power but are constrained by thermal load, rigidity, and limited scalability toward dense stimulation arrays [2]. In this work, we investigate organic light-emitting diodes (OLEDs) as alternative light sources for next-generation oCIs. Bottom-emitting OLEDs were fabricated and experimentally characterized with respect to spectral emission, efficiency, and achievable optical power density. The micro-cavity was designed by complementary optical simulations to generate a forward-directed, spatially confined illumination capable of efficiently reaching the intended spiral ganglion neurons. An implant design is proposed based on the geometry of the cochlea, required pixel size, and spacing. The combined experimental and simulation results establish OLEDs as promising alternatives to micro-LEDs for integration into future oCI architectures.

[1] A. Huet et al., Annu. Rev. Neurosci. 47, 103 (2024).
[2] L. Jablonski et al., J. Neural Eng. 22, 046034 (2025).

HL 20.58 Tue 18:00 P1

Creation and characterization of color centers in hexagonal Boron Nitride — •Dennis Heinz Bruno Mors[1,2], Iris Niehues[1], and Daniel Wigger[3] — [1]Institute of Physics, University of Münster, 48149 Münster, Germany — [2]Faculty of Science and Technology, University of Twente, 7522 NB Enschede, Netherlands — [3]Department of Physics, University of Münster, 48149 Münster, Germany

Color centers (CCs) in hexagonal boron nitride (hBN) are promising candidates for stable and bright quantum light sources, despite their unknown origin due to their single-photon emission properties even at room temperature. To explore their potential, we investigate various material sources for their ability to host CCs. We employ mechanical exfoliation to reduce the thickness of bulk crystals to a few layers, resulting in thin hBN flakes that are then transferred onto Si or SiO_2 samples. To enhance the yield of CCs, we thermally anneal the hBN. We then examine our samples using confocal photoluminescence to identify the CCs in the host crystal. Additionally, we utilize a scattering-type scanning near-field optical microscope (sSNOM) to study the photoluminescence (PL) emission characteristics of these quantum emitters. By using a sharp metallic tip, we concentrate the illuminating light field into a nanofocus, enabling us to achieve nanoscale resolution beyond the diffraction limit.[1]

[1] I. Niehues et al., Nanophotonics 2025, 14(3), 335-342.

HL 20.59 Tue 18:00 P1

Spectral wandering of single-photon emitters in the van der Waals material hBN — •Akhilesh Dubey, Robert Schmidt, Johannes Kern, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Single-photon emitters in hexagonal boron nitride (hBN) exhibit favorable photophysical optical properties at both room and cryogenic temperatures. However, their performance is limited by various line broadening mechanisms. Here, we present a low-temperature study of the photoluminescence of hBN emitters, investigating linewidth reduction and spectral diffusion at cryogenic temperatures. We believe that the spectral wandering is due to migrating charges in the vicinity of the nanoscale emitter, which could be mitigated by applying an external electric field. Our results essential for developing nanoscale quantum photonic devices based on robust hBN emitters.

HL 20.60 Tue 18:00 P1

2D Lattices of Rb Quantum Emitters on Isolating Substrates — •David Bergmann, Katharina Lorena Franzke, Wolf Gero Schmidt, and Uwe Gerstmann — Paderborn University, Paderborn, Germany

Entanglement plays a decisive role in modern application of quantum information, such as memory atoms and quantum emitters. The central challenge in this context is to address, control and protect systems of many qubits against decoherence.[1] Recently, efficient generation of entangled multiphoton graphs from single ^{87}Rb atoms was reported, overcoming the limitations encountered by probabilistic schemes.[2]

In this theoretical work, we investigate the applicability of different isolating materials to be used as substrate for a 2D lattice or clusters of ^{87}Rb atoms. In contrast to MgO, frequently used in previous investigations [3], NaCl was found to be a substrate that minimizes substrate-mediated interaction between neighboring Rb atoms. It is thus expected to allow entanglement of several individual atoms as single emitters in the same cavity. Therefore, the system Rb/NaCl promises improved scalability and opens new possibilities for quantum computation and communications.

[1] J. Preskill et al., Quantum 2, 79 (2018).
[2] P. Thomas et al., Nature 608, 677–681 (2022).
[3] R. Broekhoven et al., npj Quantum Information 10, 92 (2024)

HL 20.61 Tue 18:00 P1

Dry transfer of 2D van der Waals heterostructures for quantum sensing — •Timo Strobl, Korbinian Felber, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

A highly dynamic research area is dedicated to the development of quantum sensors based on solid-state spin defects. This field was previously focused on three-dimensional (3D) material systems, which posed challenges in positioning spin centers close to the sample surface. The recent discovery of V_B^- spin defects in the 2D van der Waals (vdW) material hexagonal boron nitride (hBN) provided a new approach to overcome this inherent positioning limitation. These defects are suitable for sensing local magnetic fields, temperature, and lattice strain when utilizing the method of optically detected magnetic resonance (ODMR). Hence, these functional hBN layers constitute a powerful tool for investigating fundamental 2D material properties.
To apply the potential in this area, the fabrication of a van der Waals heterostructure is necessary, combining the spin-active hBN with another 2D material. The precise fabrication by stacking these multilayer 2D materials via established dry-transfer polymer techniques is an essential prerequisite for such quantum sensor structures. The preparation procedures presented here provide essential insights required to implement in situ quantum sensing of 2D materials utilizing hBN.

HL 20.62 Tue 18:00 P1

Development of open-source DRC scripts for physical verification of integrated circuits with FinFET technology. — •Lev Churkin — Moscow, Russia

The development of open-source DRC scripts for FinFET technologies necessitates a fundamental shift from planar-based verification. It must encapsulate the three-dimensional nature of the transistor, enforcing complex rules for fin formation, cut patterning, and their strict alignment. Furthermore, rules must integrate with multi-patterning lithography, addressing color decomposition and spacing constraints to prevent printability errors. This requires checking more than simple geometrics. Consequently, a modern DRC script is a complex software model, which needs to manage the interdependencies of density, stress engineering, and manufacturing variability at a more advanced level.

HL 20.63 Tue 18:00 P1

Exciton dressing by extreme nonlinear magnons in a layered semiconductor — •Geoffrey M. Diederich — University of Maryland Baltimore County, 1000 Hilltop Circle, Baltimore MD, USA

Collective excitations presenting nonlinear dynamics are fundamental phenomena with broad applications. A prime example is nonlinear optics, where diverse frequency-mixing processes are central to communication and attosecond science, and extreme (>sixth-order) harmonic generation provides broad wavelength conversion. Leveraging recent progress in van der Waals magnetic semiconductors, we demonstrate nonlinear optomagnonic coupling. In the layered antiferromagnetic semiconductor CrSBr, we observe exciton states dressed by up to 20 harmonics of magnons, resulting from their extreme nonlinearities. We also create tunable optical sidebands via sum- and difference-frequency generation between two optically bright magnon modes under symmetry-breaking magnetic fields. Moreover, we can tune the observed difference-frequency generation mode into resonance with one of the fundamental magnons, which results in parametric amplification of magnons. Our findings realize the modulation of the optical-frequency exciton with the extreme nonlinearity of magnons at microwave frequencies, which could find applications in magnonics and hybrid quantum systems, and provide a method for optomagnonic neuromorphic computing devices.

HL 20.64 Tue 18:00 P1

Synthesis and characterization of new materials from the Sb-Ag-Te system — •Trayana Dolchinkova, Vladislava Ivanova, and Yordanka Trifonova — University of Chemical Technology and Metallurgy, Department of Physics, 8 Kl. Ohridski Blvd., 1797 Sofia, Bulgaria

New bulk chalcogenide materials from the Sb-Ag-Te system were synthesized by single-temperature synthesis in a closed volume. The density of the bulk samples was estimated using the pycnometer technique. Some physicochemical properties such as compactness, the molar volume and the free volume percentage of the materials were calculated, and their dependences on composition were determined. XRD analysis was performed to determine the structure and phase composition of the synthesized samples. A scanning electron microscope were used to study the surface morphology and EDS determined the chemical composition of the bulk samples.

Conclusions were drawn based on the results obtained regarding the influence of Ag content on the properties of the bulk samples.

HL 20.65 Tue 18:00 P1

Investigation of the Thermoelectric Properties of Single-Crystalline and Polycrystalline Bi1-xSbx (x =0, 0.1, 0.15) Alloys — •Fangyi Hu, Yuan Yu, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, 52074 Aachen, Germany

Thermoelectric (TE) materials can directly convert heat into electricity and vice versa, providing a sustainable and clean energy solution. Bi1-xSbx, a low-temperature n-type TE alloy with great potential between 20-200 K, has drawn increasing attention in cooling applications. Single crystals and polycrystals exhibit different performance and application prospects. In most cases, particularly below 200 K, single-crystal Bi-Sb shows much higher TE performance than polycrystals. However, polycrystalline Bi-Sb offers lower fabrication cost, better mechanical strength, and easier processing, making it attractive for large-scale use. This study compares the TE properties of Bi-Sb alloys in these two forms and clarifies their intrinsic relationship. Single-crystalline and polycrystalline Bi1-xSbx (x = 0, 0.1, 0.15) were prepared by Bridgman and melt-air-cooling methods, respectively. TE properties, with and without magnetic fields, were measured using Thermal Transport Option in a physical property measurement system (PPMS). Microstructures and bonding mechanisms were analyzed via atom probe tomography. By establishing the bonding-structure-property connection, we aim to reveal the origin of the performance difference between the two forms. These results provide insights into improving ZT in polycrystalline Bi-Sb alloys, which are more suitable for practical deployment.

HL 20.66 Tue 18:00 P1

Oxygen Vacancy-Mediated Non-Volatile Memory in RF-Sputtered Ga_2O_3 films — •Aman Baunthiyal, Jon-Olaf Krisponeit, Marco Schowalter, Alexander Karg, Andreas Rosenauer, Martin Eickhoff, and Jens Falta — Institute of Solid State Physics, University of Bremen, Bremen, Germany

To address the memory bottleneck in conventional electronics, resistive switching (RS) has emerged as a promising route for next-generation memory technologies. Among various materials used in RS devices, β-Ga_2O_3 offers advantages such as high breakdown strength and defect-mediated conductivity. However, its direct growth on metal electrodes with controlled microstructure, crucial for scalable vertical devices, remains largely unexplored. Here, we investigate RF-sputtered Ga_2O_3 deposited on smooth Ru(0001) films for non-volatile RS applications.

XRD and TEM confirm the temperature-dependent structural evolution of Ga_2O_3 and its correlation with the I–V response. Devices grown at intermediate temperatures (∼400°C) show the best switching window (up to 10^4), with thinner films enabling low set voltages (∼1.5 V) [1] but poorer stability. In contrast, thicker layers require higher voltages (∼4 V) yet offer better reliability [2]. This behaviour arises from temperature-driven grain growth and the $\gamma \rightarrow \beta$ phase transition [3], which creates mixed phases and grain boundaries that govern oxygen-vacancy-mediated filament dynamics.

[1] A. Baunthiyal *et al.*, *Appl. Phys. Lett.* **123**, 213504 (2023). [2] A. Baunthiyal *et al.*, *2023 IEEE NMDC*, pp. 536-540. [3] A. Baunthiyal *et al.*, *APL Mater.* **13**, 041130 (2025).

HL 21: Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)

Time: Wednesday 9:30–10:30 Location: HSZ/0101

HL 21.1 Wed 9:30 HSZ/0101

Locally Imaging the Insulator to Metal Transition of Ca_2RuO_4 with Single Spin Magnetometry — •Hayden Binger[1], Cissy Suen[2], Young-Gwan Choi[1], Yejin Lee[1], Haolin Jin[1], Max Krautloher[2], Yuchen Zhao[1], Luke Turnbull[1], Elina Zhakina[1], Jeffrey Neethirajan[1], Lotte Boer[1], Berit Goodge[1], Piotr Surówka[3], Roderich Moessner[4], Bernhard Keimer[2], Claire Donnelly[1], and Uri Vool[1] — [1]MPI CPfS, Dresden, Germany — [2]MPI FKF, Stuttgart, Germany — [3]Wrocław University of Science and Technology, Wrocław, Poland — [4]MPI PKS, Dresden, Germany

The current-driven insulator to metal transition (IMT) in Ca_2RuO_4 is a fascinating phenomenon where increasing current driven across a sample causes a smaller voltage difference to develop. We have created devices of size 10-20 um by 10-20 um and 100 nm thick using Focused Ion Beam (FIB) milling. Through the utilization of Nitrogen Vacancies (NV), optically addressable spin-1 defects acting as a qubit at room temperature, we probe the local magnetic field at the defect via the Zeeman interaction. We are thusly able to image the local character of the insulator to metal transition in Ca_2RuO_4. At low currents we image the formation of a singular conducting channel at the edge of the device, which gradually grows throughout the entire device as more current is applied until eventually current flows evenly across the device. We explore reasons why local current channels nucleate at the edge, such as strain, defects, and crystalline lattice orientation.

HL 21.2 Wed 9:45 HSZ/0101

Topological Ambiguity in Stray Field Magnetometry — •Shirsopratim Chattopadhyay[1,2] and Aparajita Singha[1,2] — [1]IFMP, TU Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence (ct.qmat)

Inferring magnetic topology from stray field measurements is central to characterizing skyrmions, vortices, and other topological textures. Yet, the uniqueness of such reconstructions remains poorly characterized. We present a computational framework to systematically generate pairs of magnetization configurations with distinct topological charges ($|\Delta Q| = q$, where q can be set by the user) that produce nearly identical stray fields (Normalized Root Mean Square Error ~ 0.8-4 percent). Our approach uses constrained optimization with a physics informed loss to jointly evolve magnetization pairs towards field degeneracy while preserving topological distinction. Across 200 randomized trials with varied initializations, we demonstrate rapid and reliable generation of adversarial pairs spanning skyrmions, merons, fractional defects and uniform domain textures. We theoretically analyse the relation between topological charge and stray field and construct an explicit example of near identical stray field from distinct topologies. Our adversarial dataset enables rigorous assessment of magnetization reconstruction algorithms and guides the design of measurement strategies capable of resolving topological ambiguity.

HL 21.3 Wed 10:00 HSZ/0101

Towards Cryogenic Scanning Nitrogen Vacancy Magnetometry — •Lotte Boer[1], Kilian Srowik[1], Hayden Binger[1], Young-Gwan Choi[1], Ahmet Ünal[1], Edouard Lesne[1], Matheus Barbosa[2], Bernd Büchner[2], Alexey Popov[2], and Uri Vool[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW Dresden, Germany

In scanning nitrogen vacancy (NV) magnetometry, an atomic force microscopy tip is replaced with a diamond pillar containing a single NV center, which acts as a highly sensitive magnetic field sensor. Scanning over a sample then allows to map the magnetic stray field. This method has been widely used at room temperature to investigate, for example, magnetic textures in thin films or local current flow patterns. However, a wide range of interesting material properties, such as emergent magnetic phases and superconductivity only occur at lower tempera-

tures. As the NV center retains its ability to sense magnetic fields at low temperatures, we are developing a variable temperature cryogenic scanning NV system. This will not only allow for the imaging of materials at low temperatures, but also allow for the unique opportunity of mapping magnetic phase transitions in quantum materials.

Building a cryogenic NV setup presents several challenges, as the NV requires optical access for readout and microwave pulses for control, all within tight spatial confines and while preventing sample heating. In this talk, we will discuss our setup, which is in its final stages of development, and show preliminary measurement results at few Kelvin temperatures.

HL 21.4 Wed 10:15 HSZ/0101

CISS from Vibrationally Assisted Tunneling in Chiral Molecules — •Fedor Baranov, Virginia Gali, and Maxim Breitkreiz — Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany

Chiral-induced spin selectivity (CISS) remains a puzzling phenomenon, despite extensive experimental evidence. A possible explanation emerges when recognizing that charge transport through chiral insulating molecules occurs in the tunneling regime, where even small spin-orbit coupling becomes crucial inside the barrier. This enhancement leads to a spin-dependent potential that gives different tunneling probabilities for different spin orientations. Because this tunneling alone produces extremely small currents, one has to take into account the vibrational degrees of freedom of the system that in the static limit increases the current while preserving the spin splitting nature. Together, these ingredients offer a transparent physical mechanism underlying the CISS effect.

HL 22: Biocompatible Organic Semiconductors

Time: Wednesday 9:30–11:00 Location: POT/0006

HL 22.1 Wed 9:30 POT/0006

Stable n-Type OECTs with BBL: Unlocking Complementary Circuits — •Clemens Rössler[1,2], Laura Teurle[1,2], Hans Kleemann[1,2], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials — [2]TU Dresden

Organic mixed ionic-electronic conductors (OMIECs) have emerged as a key materials platform for next-generation bioelectronics, energy-efficient signal processing, and neuromorphic computing. Among the most versatile OMIEC devices is the organic electrochemical transistor (OECT), whose ability to couple ionic and electronic transport enables low-voltage operation and is particularly advantageous for solid-state electrolyte systems that enable densely integrated circuitry. While p-type materials such as PEDOT:PSS have driven much of the field's progress, the lack of stable and high-performance n-type counterparts remains a critical bottleneck - limiting the realization of complementary circuits, low-power logic, and more complex bioelectronic architectures. In this talk, I present recent progress on n-type OECTs based on the ladder polymer poly(benzimidazobenzophenanthroline) (BBL). I will discuss how we have developed and optimized n-type OECTs that exhibit remarkable stability and a unique electrochemical conditioning behaviour. Spectroscopic, AFM, and transfer curve analyses show that BBL combines excellent optical and morphological stability with a high mobility capacitance product, indicating efficient ion penetration and intrinsically high electronic mobility.

HL 22.2 Wed 9:45 POT/0006

A Nonlinear Organic Infrasound Sensor — •Maarten Mittmann[1], Carsten Habenicht[1], Andreas Hofacker[1], Richard Kantelberg[1], Stefan Jacob[2], Hans Kleemann[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Dresden University of Technology, 01062 Dresden, Germany — [2]National Metrology Institute (PTB), 38116 Braunschweig, Germany

Most works on speech recognition using reservoir computing focus on the nonlinear transformation of the data, which is fed electronically from a conventional sensor to the device. However, this approach necessitates two separate devices, consuming power and possibly requiring additional signal processing steps. In this work, we demonstrate that an efficient interface between acoustic stimulation and nonlinear, electronic output can be established using a free-standing viscoelastic film containing a poly(3,4-ethylenedioxythiophene) hexafluorophosphate (PEDOT:PF_6) fiber organic electrochemical transistor (OECT). Upon application of a constant drain-source and gate-source voltage, the system shows a time-dependent, nonlinear modulation of the drain current when excited acoustically. This nonlinearity opens possibilities of combining the existing system with a reservoir computing approach to perform complex tasks like infrasound source discrimination and anomaly detection. The devices show great sensitivity within the order of magnitude of $10^2\ mV\ Pa^{-1}$ in the infrasound frequency regime thanks to the amplification via the gate electrode.

HL 22.3 Wed 10:00 POT/0006

Is Printed Electronics a Sustainable Technology? A Framework to Efficiently Implement an Early-Stage Life-Cycle-Analysis — •Laura Teuerle, Tommy Meier, Klara Hänisch, Finn Jaekel, Yeohoon Yoon, Andreas Wendel, and Hans Kleemann — Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Germany

The rise of microelectronic system has been the major driving focus of the global economy for the last couple of decades. As we are now transitioning to the era of the internet-of-things, with an increasing number of small autonomous electronic circuits, e.g, for sensing, we need to urgently consider the environmental impact of this development due to the unsustainable use of natural resources. Thus, to ensure the environmental sustainability of the development, future electronics must prioritize both performance and environmental impact, explaining the interest in flexible and printed electronics. However, the sustainability claims often connected to the field of flexible and printed electronics must be substantiated using analytic methods, providing the motivation for quantitative Life-Cycle Assessment (LCA). Here we demonstrate our approach to implement an LCA for an early-state research topic such as Organic Electrochemical Transistors (OECTs). Using hands-on examples, we will show how to set up an inventory database (the core of the LCA) using a process-of-record (PoR). By making LCA a standard tool in printed electronics, the community can move beyond sustainability claims to measurable environmental impact, driving truly responsible innovation in electronics.

HL 22.4 Wed 10:15 POT/0006

Obtaining In-Vivo Data for AI Applications Using Implantable Biocompatible Materials — •Finn Jaekel[1], Richard Kantelberg[1], Hans Kleemann[1], Daniel Freund[2], Julia Henne[2], Dennis Wahl[2], Eberhard Grambow[3], Sebastian Hinz[2], Clemens Schafmayer[2], Jochen Hampe[4], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — [2]Klinik und Poliklinik für Allgemeine Chirurgie, Thorax, Gefäß- und Transplantationschirurgie, Universitätsmedizin Rostock, Rostock, Germany — [3]Klinik für Herz-, Thorax- und Gefäßchirurgie (HTG), Universitätsmedizin Göttingen, Göttingen, Germany — [4]Universitätsklinikum Carl Gustav Carus Dresden, Dresden, Germany

Artificial intelligence can be of great use in biomedical applications, especially when implemented in implantable hardware solutions. However, robust, biomedical AI applications crucially depend on real, high-quality, physiological training and input datasets, which are scarce in practice. In this presentation, we provide a prototypical use-case scenario by demonstrating in-vivo impedance measurements in a porcine small-intestinal anastomosis using printed, fully biocompatible organic sensors. Ischemia was induced locally, and manual evaluation shows a characteristic signature in the recorded impedance spectra, confirming that the system captures physiologically relevant data. This positions the technology in a realistic sensor to AI analysis pipeline, where automated detection of ischemia can be used to create an early warning system of anastomotic failure.

HL 22.5 Wed 10:30 POT/0006

Towards Fully Biodegradable and Sustainable Organic Electrochemical Transistors Printed on Leaf-Derived Substrates — •Bilge Kahraman, Rakesh R. Nair, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and

Photonic Materials, Technische Universität Dresden, 01187 Dresden, Germany.

The rapid proliferation of disposable electronics has exacerbated electronic waste and its associated environmental burden. Here, we demonstrate fully screen-printed organic electrochemical transistors (OECTs) fabricated on robust biodegradable leaf-derived substrates using non-toxic carbon and PEDOT:PSS-based inks. Magnolia grandiflora leaves were skeletonized to function as sequestering matrices for hydroxypropylcellulose (HPC) based resin, which was subsequently crosslinked to create robust flexible, compostable substrates. Life-cycle assessment (LCA) reveals that the combination of leaf-skeleton-based substrates and carbon gate electrodes for electronic device fabrication reduces CO_2-equivalent emissions by up to four orders of magnitude compared to conventional glass substrates and gold electrodes (19,400 times lower for substrates; 680 times lower for electrodes). The printed OECTs exhibit steady-state performance comparable to devices made on glass using commercial PEDOT:PSS formulations, with on/off ratios $> 10^4$ and transconductance values exceeding 1 mS. This work presents a viable path toward truly green bioelectronic devices that can be manufactured for disposability and safely returned to the environment after use.

HL 22.6 Wed 10:45 POT/0006

Flexible Organic Photodiodes Based on Advanced Encapsulation Strategies — •Rabiul Islam[1,2], Siddhartha Saggar[1,2], Jakob Wolansky[3], Darius Pohl[4], Markus Löffler[4], Bernd Rellinghaus[4], Johannes Benduhn[3], and Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, Technische Universität Dresden, Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, Waldheim, Germany — [3]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [4]Dresden Center for Nanoanalysis (DCN), Technische Universität Dresden, Dresden, Germany

Organic photodiodes (OPDs) are promising for biomedical applications due to their flexibility, spectral tunability, and biocompatibility, yet their moisture sensitivity demands robust encapsulation for long-term operation. Conventional flexible substrates offer limited device protection in humid conditions; to overcome this, we employed a parylene-C/ALD-deposited Al2O3/ZrO2 hybrid substrate, providing flexibility and strong barrier properties. We fabricated flexible OPDs with an ultrathin (7 nm) silver electrode on a hybrid substrate, which remained stable after 10,000 bending cycles and demonstrated high mechanical robustness. Using PM6:PC71BM as the active layer, the OPDs achieved responsivity of 0.26 A/W at -0.1 V under 639 nm illumination, retained 86% of their initial performance after 12 days in deionized water, and remained functional after one hour of machine washing, showing that parylene/nanolaminate-based ultra-flexible OPDs enable long-term operation in aqueous environments.

HL 23: Transport Properties

Time: Wednesday 9:30–12:15 Location: POT/0051

HL 23.1 Wed 9:30 POT/0051

Nonlinear charge transport in single crystalline slabs of Bi2Se3 — •Igor Veremchuk[1], Pavlo Makushko[1], Anita Guarino[2], Muhammad Waqee Ur Rehman[2], Rosalba Tatiana Fittipaldi[2], Tobias Kosub[1], Alexej Pashkin[1], Fabian Ganss[1], Proloy T. Das[1], Rui Xu[1], Rhonald Burgos Atencia[3], Debottam Mandal[3], Antonio Vecchione[2], Carmine Ortix[3,2], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]CNR-Institute for SuPerconductors, Innovative materials, and devices, Salerno, Italy — [3]Dipartimento di Fisica "E. R. Caianiello", Universita di Salerno, IT-84084 Fisciano (SA), Italy

Nonlinear charge transport is central to next-generation high-frequency electronics, enabling efficient rectification and frequency conversion up to the THz range. Nonlinear responses are observed in various material systems often focusing on thin films including Bi [1], Te [2], and Bi2Se3 [3]. In this study, we will report experimental observations of nonlinear charge transport in Bi2Se3 single crystals, which is explained based on peculiarities of the structural properties of layered Bi2Se3 materials. Our findings can be applied to a broad range of van der Waals centrosymmetric compounds.

[1] P. Makushko, I. Veremchuk et al., Nat. Electron. 7, 207 (2024).
[2] B. Cheng et al., Nat. Commun. 15, 5513 (2024).
[3] P. He et al., Nat. Commun. 12, 698 (2021).

HL 23.2 Wed 9:45 POT/0051

Comparing thermal conductivity predictions from open source phonon transport solvers — •Sally Issa, Martí Raya-Moreno, and Nakib H. Protik — Humboldt-Universität zu Berlin, Germany

Phonon transport continues to be an active field of research, both for probing materials physics and developing applications for thermoelectricity and thermal management. Due to their parameter-free nature, ab initio approaches are one of the preferred means for solving the phonon transport problem, offering excellent predictive capabilities, especially for novel materials. Over the last decade, the workflow combining density functional theory (DFT) and the Peierls Boltzmann transport equation (BTE) has gained popularity. Indeed, practitioners in the field have several publicly available BTE code packages to choose from, for example, ShengBTE, AlmaBTE, phonop3py, elphbolt, Phoebe, etc., that use this workflow. Nevertheless, the doubt regarding the comparability of these different codes still remains. At present, a detailed comparative study is missing in the literature. In this work, we fill this gap and carry out a comparison of the phonon thermal conductivity predicted by various codes. For a fair comparison, we use the same DFT generated interatomic force constants from the Alma database [1] for all considered codes. We carefully check the convergence of the thermal conductivity with respect to the wave vector mesh density and compare the results over a range of temperature points.

[1] ALMA database: https://almabte.bitbucket.io/database/

HL 23.3 Wed 10:00 POT/0051

Influence of Thermal Annealing on CMOS-Integrated Graphene Field-Effect Transistors — •Daniel Nickel[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP - Leibniz Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

This work investigates the influence of consecutive annealing on CMOS-integrated graphene field-effect transistors (GFETs) with annealing temperatures (T_a) from 150 °C up to 300 °C. The GFETs were fabricated on 200 mm SiO_2/Si wafers with Pd/Au and Ni edge contacts, tungsten backgate and Si_3N_4 passivation. Annealing was carried out in 150 sccm nitrogen flow for 1 h using a 10 °C/min ramp. Electrical transfer measurements show that maximum p- and n-type field-effect mobilities occur at T_a = 200 °C for Pd/Au ($\mu_p \approx 950$ cm^2/Vs, $\mu_n \approx 1650$ cm^2/Vs) and at T_a = 150 °C for Ni ($\mu_p \approx 450$ cm^2/Vs, $\mu_n \approx 890$ cm^2/Vs). Raman analysis indicates an improved graphene quality with increasing T_a. Raman mapping reveals that for Pd/Au, the FWHM of the 2D peak reaches a minimum at $T_a = 200$ °C, followed by a slight increase in compressive strain at higher T_a. For Ni, broader 2D and G peak distributions and a reduction in p-doping with increased T_a is observed. Raman data measured near the Ni contacts reveal reduced p-doping, whereas doping near the Pd/Au contacts remains largely unaffected. Funding was provided by EU Horizon 2020 Graphene Flagship grants 101189797 and 101120938.

HL 23.4 Wed 10:15 POT/0051

Elucidating mobile charge carriers in granular matter by transient surface photovoltage analysis — •Christoph Merschjann[1], Albert These[2], Christoph Brabec[2,3], Thomas Dittrich[1], and Pablo Jimenéz-Calvo[2,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen — [3]Helmholtz-Institute Erlangen-Nürnberg, Erlangen — [4]Max-Planck-Institute of Colloids and Interfaces, Potsdam

Among the most important properties of novel functional materials are their charge transport characteristics, including n vs. p type conduc-

tivity, carrier concentrations, and respective mobilities. However, new solid-state materials are typically first synthesized in granular form, and often this is also the intended morphology for applications (batteries, photocatalysts, etc.). This makes most electrical characterization techniques (e.g. impedance, Hall, time-of-flight photocurrent) extremely challenging, as they rely on current measurements throughout the bulk of the sample. To overcome this drawback, we use contactless transient surface photovoltage (TR-SPV) to detect charge-density shifts on the nanometer scale and in a time range from nanoseconds to seconds. Comparing the results with diffusive charge-transport models of moderate complexity, we are able to deduce the type and mobility of photoinduced charge carriers in a prominent example material, graphitic polymeric carbon nitride (PCN). We encourage transferability of this SPV analysis to other 2D layered systems like metal- or covalent-organic frameworks (MOF / COF).

HL 23.5 Wed 10:30 POT/0051

Deep-learning Hamiltonian Acceleration of Electrical Transport Predictions using the Non-Perturbative *ab initio* Kubo-Greenwood Method for Strongly Anharmonic Materials — •Juan Zhang[1,2], Kisung Kang[3], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin — [2]Department of Optical Science and Engineering, Fudan University, Shanghai — [3]School of Materials Sciences and Engineering, Chonnam National University, Gwangju

Thermal insulators, e.g., needed for efficient thermoelectric materials, feature strong anharmonicity. As a consequence, a perturbative approach of electron-phonon interactions and even the phonon concept for describing vibrations may become invalid. The non-perturbative *ab initio* Kubo-Greenwood (aiKG) method provides an approach for evaluating electron and hole mobilities [1]. However, it requires substantial computational costs due to its high requirements with respect to statistical averages, large supercells, and extrapolation strategies to the zero-frequency limit. This work introduces an AI-assisted aiKG framework for the FHI-aims code, which incorporates the neural-network model, DeepH [2], trained to predict the Kohn-Sham Hamiltonian. Using the thermal insulator KI, we demonstrate the capabilities and predictive power of the approach, which substantially accelerates the calculation of large supercell electronic band structures, temperature-dependent spectral functions, and carrier mobilities with high accuracy.

[1] J. Quan *et al.* Phys. Rev. B 110, 235202 (2024).
[2] X. Gong, *et al.* Nat Commun 14, 2848 (2023).

HL 23.6 Wed 10:45 POT/0051

Quantum oscillations in the correlated metal $CaVO_3$ — Olivio Chiatti[1], Mahni Müller[1], Maria Espinosa[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and •Saskia F. Fischer[1,4] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Transparent conductive materials are in great demand in the optoelectronic industry for their high-performance and cost-effectiveness. Strong electron-electron interactions in correlated metals can enhance the carrier effective mass and allow to achieve both high-optical transparency and high-electrical conductivity [1].

Here, we study the electric transport properties of thin $CaVO_3$ epitaxial films grown on $LaAlO_3$ substrates by hybrid molecular beam epitaxy, with residual a high resistivity ratio (RRR) up to 98 [2]. Magnetortransport measurements were performed between 2 and 200 K in magnetic fields up to 64 T. Films with high RRR show quantum oscillations below 10 K. The analysis of the Shubnikov-de Haas oscillations provides parameters within a multi-carrier model and the implications for the complex Fermi surface of $CaVO_3$ are discussed.

[1] Zhang *et al.*, Nature Materials **15**, 204 (2016)
[2] Kuznetsova *et al.*, APL Materials **11**, 041120 (2023)

15 min. break

HL 23.7 Wed 11:15 POT/0051

Modeling the impact of dynamic disorder on optical conductivity of semiconductors using a Kubo approach — •Frederik Vonhoff[1], Michel Panhans[2], David R. Reichman[3], Frank Ortmann[2], and David A. Egger[1] — [1]Physics Dep., TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Dep. of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Dep. of Chemistry, Columbia University, New York, NY 10027, USA

Semiconductor devices rely critically on efficient charge-carrier transport, making it essential to understand the underlying transport mechanisms. The optical conductivity is a key transport observable, both experimentally and theoretically, for identifying the scattering mechanisms and transport regimes. However, modeling the transport properties of semiconductors with strong nuclear vibrations is challenging due to the resulting dynamic disorder in the electronic structure [1, 2]. Addressing these challenges, we develop a dynamic-disorder-driven microscopic method to compute optical conductivities in one- and three-dimensional semiconductor model systems by integrating time-dependent electronic Hamiltonians in Kubo transport theory. By systematically varying the static and dynamic disorder strength, we investigate the transition from localization to transient localization to and diffusive behavior, providing insights into scattering mechanisms active in emerging semiconductor materials such as halide perovskites.

[1] J. Fetherolf, et al, Physical Review X 10, 021062 (2020)
[2] F. Vonhoff, et al, Physical Review Materials 9, 094601 (2025)

HL 23.8 Wed 11:30 POT/0051

Self-Trapped Exciton Diffusion in a Lead-Free Two- Dimensional Hybrid Perovskite — •Jan-Heinrich Littmann[1], Lukas Gümbel[1], Philip Klement[1], Meng Yang[2], Markus Stein[1], Johanna Heine[2,3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Hans-Meerwein- Straße, 35043 Marburg, Germany — [3]Institute of Chemistry, Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, 26129 Oldenburg, Germany

Self-trapped excitons (STEs) in low-dimensional metal-halide perovskites arise from lattice distortions. The mobility of such excitations is expected to be limited, however, remains vastly unexplored experimentally.

Here, we directly image STE transport in a lead-free perovskite using spatially and temporally resolved photoluminescence microscopy. The STEs exhibit measurable mobility and propagate over micrometer distances despite their strongly-localized nature. At low temperatures, their motion is limited and nearly temperature independent. Transport becomes thermally activated above 150k and overcomes local energy barriers. Together this infers trap-limited diffusion. These results establish that STEs are mobile under suitable conditions and provide a quantitative framework for STE transport in lead-free perovskite materials.

HL 23.9 Wed 11:45 POT/0051

Electron-phonon interactions in VASP — •Manuel Engel[1], Henrique Miranda[1], Atsushi Togo[2], Laurent Chaput[3], Martijn Marsman[1], and Georg Kresse[1,4] — [1]VASP Software GmbH, Vienna, Austria — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Lorraine University, Nancy, France — [4]University of Vienna, Vienna, Austria

Understanding electron-phonon interactions with first-principles accuracy is essential for predicting temperature-dependent electronic properties in semiconductors and complex materials. In this work, we present new capabilities implemented in VASP that enable a fully ab initio treatment of electron-phonon coupling using the projector-augmented wave (PAW) method. These developments provide a consistent framework for evaluating band-gap renormalization, phonon-induced linewidths, and finite-temperature electronic transport properties within density functional theory.

Our approach combines perturbative electron-phonon matrix elements with dense Brillouin-zone sampling achieved through interpolation techniques compatible with PAW-based orbitals and higher-level density functionals. We demonstrate accurate predictions of zero-point and thermal band-gap shifts across a range of materials. In addition, we incorporate the electron-phonon scattering rates directly into Boltzmann transport calculations under relaxation-time approximations. This enables temperature-dependent mobilities and conductivities to be computed from first principles.

HL 23.10 Wed 12:00 POT/0051

Investigation of exciton diffusion in GaAs nanowires via cathodoluminescence spectroscopy — •Mikel Gómez Ruiz,

Vladimir Kaganer, Jesús Herranz, Lutz Geelhaar, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Semiconductor nanowire (NW) structures emitting at tailored wavelengths have attracted notable interest for integration with silicon-on-insulator waveguides. For many of these applications, the efficiency with which carriers are injected into the active region of the sample is relevant.

In this context, carrier transport in phase-pure GaAs nanowires is investigated by spatially-resolved cathodoluminescence spectroscopy. Emission intensity profiles along the nanowire axis are measured to study carrier transfer from the GaAs segment to the axial interfaces at both ends of the nanowire. These interfaces are formed at the top with the axially grown (Al,Ga)As shell and at the bottom with the Si substrate. The recorded intensity profiles are predominantly asymmetric, indicating that carrier recombination at the two interfaces occurs in a different fashion.

These profiles are analyzed using a mathematical model that accounts for carrier generation, diffusion, and recombination. Fitting this model to the experimental profiles reveals a diffusion length exceeding one micron at 10 K, an unprecedented value for GaAs nanowires. This reflects the high crystal quality of our nanowires.

HL 24: 2D Materials IV – Emerging materials and properties

Time: Wednesday 9:30–12:45 Location: POT/0081

HL 24.1 Wed 9:30 POT/0081

Atomic layer deposition of few-layer 1T-TiS_2 and ternary $MoTiS_2$ — •Christian Petersen[1,2], Christian Tessarek[1,2], Marco Schowalter[1,2], Andreas Rosenauer[1,2], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany

Theoretical calculations and experimental data concerning electronic and structural properties of 1T-TiS_2 are sparse in comparison to other transition metal dichalcogenides (TMD) such as MoS_2. The available data is contradicting and attributes 1T-TiS_2 a plethora of different properties ranging from a semi-metal like behaviour to different charge density wave phases (2×2 and $\sqrt{7} \times \sqrt{3}$) and even a band gap of up to 2.5 eV. In general, there is a lack of experimental data due to difficulties in synthesis and stabilization of 1T-TiS_2 which rapidly oxidizes in ambient conditions.

In this study, plasma-enhanced sub-atomic layer deposition (ALD) [1] in combination with in situ X-ray photoelectron spectroscopy (XPS) is employed to directly study the effects of the growth conditions on the chemical composition of 1T-TiS_2 while circumventing the problem of oxidation in ambient. To further characterize the 1T-TiS_2 film ex situ, Raman spectroscopy and atomic force microscopy (AFM) is utilized. Additionally, $MoTiS_2$ was synthesized by substitution of ALD cycles of the Ti precursor (TDMAT) by the Mo precursor (BTBMMo).

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

HL 24.2 Wed 9:45 POT/0081

The effect of Lithium intercalation on line defects in the MoS2 monolayer — •Asghar Ali Jan and Peter Kratzer — University of Duisburg-Essen, Duisburg, Germany

MoS2 can be an effective anode material in lithium-ion batteries, as it is scalable at room temperature and has weak van der Waals forces, allowing lithium ions to intercalate between the sheets. Additionally, when using MoS2 as an anode in a lithium-rich environment, the phase transition from the most stable H phase to the T' phase must also be considered. Certain defects, such as sulfur vacancies and grain boundaries, are often present in experimentally synthesized MoS2 layers. These grain boundaries introduce metallic states within the bulk band gap. As a result, the conductivity of MoS2 is reduced. Up to now, the H-to-T' phase transition in MoS2 has been extensively studied, but generally without considering the possible presence of defects such as grain boundaries. Therefore, we have investigated the interaction of lithium intercalation with the grain boundaries present in a MoS2 monolayer. For example, we examine how the presence of lithium near a mirror twin boundary (MTB) affects the one-dimensional line of charge trapped in the MTB. It is also important to consider the grain boundary formed when a T' phase created from the H phase due to lithium intercalation directly meets the remaining H phase that does not interact with lithium. Our density functional theory calculations provided insights about the stability and electronic properties of these line defects in the presence of lithiation.

HL 24.3 Wed 10:00 POT/0081

Wafer-scale growth of hexagonal boron nitride thin films using pulsed laser deposition — •Daniel Klenkert[1,2], Benedikt Winter[1], Paul Konrad[2], 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 Würzburg, 97074 Würzburg

Hexagonal boron nitride (hBN) has attracted significant attention due to its wide bandgap, high thermal conductivity and its ability to host optically active defects, which are promising as single photon emitters and for quantum sensing applications. Thus far the sample preparation of hBN usually relies on tape exfoliation or high temperature chemical vapor deposition. Here we report on our progress using an alternative approach to prepare thin films of hBN on different substrates: pulsed laser deposition. This enabled the preparation of microcrystalline hBN layers on large scale wafer substrates at temperatures below 850°C. The stoichiometry preserving properties of pulsed laser deposition also allows for the preparation of carbon doped thin films. These are especially interesting for research on carbon related, optically active defects, which are noted for their high brightness and single photon purity.

HL 24.4 Wed 10:15 POT/0081

Doping-Induced Modulation of Structural and Electronic Properties in Transition Metal Dichalcogenides — •Cem Sanga[1,3], Nadire Nayir[1,3], Yusuf Kerem Bostan[2], Fahrettin Sarcan[2], Diwakar Singh[4], and Tanushree Choudhury[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Physics, Faculty of Science, Istanbul University, Vezneciler, Istanbul, 34134, Turkey — [3]Department of Physics Engineering, Istanbul Technical University, Maslak, Istanbul, 34467, Turkey — [4]Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, Maharashtra 400076, India

Transition metal dichalcogenides (TMDCs) hold promise for electronic applications, yet their performance is limited by inadequate doping strategies. This density functional theory investigation examines substitutional and interstitial doping in MoS_2 and WS_2 using chlorine and oxygen dopants. Formation energy calculations reveal chlorine preferentially occupies sulfur vacancy sites in MoS_2. Electronic structure analysis demonstrates that strategic doping enables bandgap engineering in TMDC systems.

HL 24.5 Wed 10:30 POT/0081

Opposite In-Plane Electrical Anisotropy in $ZrSe_3$ and ZrS_3 Flakes — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hannover, Germany

The anisotropy in form of quasi one-dimensional (1D) chains in transition metal trichalcogenides (TMTCs) makes them stand out compared to other more conventional two-dimensional (2D) materials [1]. Through width-dependent [2] and direct measurements, we investigated the electrical properties of $ZrSe_3$ and ZrS_3 flakes, in particular, the influence of the anisotropic effective electron masses [3] in the 2D plane. Flakes with a height of 26 nm were exfoliated from the respective bulk materials grown by a chemical vapour transport method.

Despite their identical quasi 1D layered crystal structure, $ZrSe_3$ and

ZrS_3 exhibits inverted in-plane electrical anisotropy. While $ZrSe_3$ exhibits the highest conductivity across the 1D chains with an anisotropy ratio of 0.60, ZrS_3 is shown to favour electron transport along the 1D chains with a ratio of 1.69. Using DFT, we attribute this to the different chalcogen contributions at the conduction band minimum.

[1] J. O. Island et al., 2D Materials 4, 0220033 (2017)
[2] D. Höllmann et al., ACS Appl. Electron. Mater. 7, 9, 4049-4054 (2025)
[3] Y. Jin et al., Phys. Chem. Chem. Phys. 17, 18665-18669 (2015)

HL 24.6 Wed 10:45 POT/0081

Observation of Bernal Stacking in Few-Layer Graphene on C face Silicon Carbide — •Jonas Rose, Oliver Brandt, Michael Hanke, Joao Marcelo Lopes, Philipp John, and Hans Tornatzky — Paul-Drude-Institut, Berlin

Epitaxial growth of few-layer graphene (FLG) on SiC(000$\bar{1}$) (C face) is widely assumed to yield films with rotational disorder, in contrast to the well-ordered Bernal (AB) stacking typically associated with SiC(0001) (Si face) growth. In this work, we show that surface graphitization on the C face of SiC can, under appropriate conditions, produce FLG with genuine AB stacking and remarkably low mosaic spread. Using detailed Raman spectroscopy, supported by complementary structural characterization, we identify clear spectral signatures of Bernal ordering, including a well-defined 2D-band lineshape. These findings demonstrate that ordered stacking is achievable on the C face under controlled sublimation conditions. We will present our full spectroscopic analysis and discuss its implications for the structural and electronic properties of the grown FLG.

15 min. break

HL 24.7 Wed 11:15 POT/0081

Influence of Defects, Doping and Layer Twisting on Phonon Dispersions in Bilayer Graphene and MoS_2 from Machine-Learned Force Fields — •Sabuhi Badalov and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

In two-dimensional (2D) layered materials, phonon dispersion plays a central role in determining transport and electronic properties. In bilayer systems, phonon dispersion is highly sensitive to the stacking configuration, twist angle, defects, and doping types. Using *state-of-the-art* machine learning force fields trained on the *first-principles* data, we perform large-scale phonon calculations for bilayer graphene and MoS_2 to investigate how layer twist and defect density alter phonon spectra and interlayer vibrational modes. We also analyze the influence of p- and n-type doping on phonon dispersions and their interactions with the underlying electronic structure. Our results reveal characteristic shifts in low-energy acoustic and optical branches that are directly linked to microscopic structural motifs, including *Moiré*-induced phonon properties. These findings provide microscopic input for future calculations of electron-phonon coupling and possible phonon-mediated superconducting states in twisted and doped 2D materials and establish machine learning force fields as a powerful framework for exploring phonon-electron interaction in quantum materials.

HL 24.8 Wed 11:30 POT/0081

Efficient *GW* band structure calculations using Gaussian basis functions and application to atomically thin transition-metal dichalcogenides — •Rémi Pasquier[1], María Camarasa-Gómez[2,3], Anna-Sophia Hehn[4], Daniel Hernangómez-Pérez[5], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain — [3]Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Química, UPV/EHU, 20018 Donostia-San Sebastián, Spain — [4]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Strasse 1, 24118 Kiel, Germany — [5]CIC nanoGUNE BRTA, Tolosa Hiribidea 76, 20018 San Sebastián, Spain

The *GW* approximation is widely used to compute self-energies and related electronic properties but remains computationally demanding, motivating the development of more efficient approaches. We present a space-time *GW* algorithm for periodic systems in a Gaussian basis with spin-orbit coupling, enabling accurate and efficient quasiparticle band-structure calculations for atomically thin materials. For monolayer MoS_2, $MoSe_2$, WS_2, and WSe_2, the resulting *GW* band gaps agree on average within 50 meV with plane-wave reference values. Full G_0W_0 band structures can be computed in less than two days on a laptop (Intel i5, 192 GB RAM) or under 30 minutes using 1024 cores.

HL 24.9 Wed 11:45 POT/0081

Investigating the Ferroelectric Potential Landscape of 3R-MoS_2 through Optical Measurements — •Jan-Niklas Heidkamp[1], Johannes Schwandt-Krause[1], Swarup Deb[1,2,3], Takashi Taniguchi[4], Kenji Watanabe[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Homi Bhabha National Institute, Mumbai, India — [3]Saha Institute of Nuclear Physics, Kolkata, India — [4]National Institute for Material Science, Tsukuba, Japan

In recent years, sliding ferroelectricity has emerged as a topic of significant interest due to its possible application in non-volatile, reconfigurable storage devices. This phenomenon is unique to two-dimensional van der Waals materials, where out-of-plane ferroelectric polarization switching is induced by relative in-plane sliding of adjacent layers. The intrinsic stacking order influences the resulting polarization, creating distinct polarization regions separated by domain walls. These can be manipulated using an applied vertical electric field, enabling a switchable system that retains the environmental robustness of van der Waals materials. This study investigates 3R-MoS_2 using various optical measurement techniques at room temperature and reveals apparent signal changes corresponding to different ferroelectric stacking orders and variations in layer count. Our findings demonstrate that fast optical mapping at room temperature is a reliable method for probing ferroelectric potential steps in 3R-stacked MoS_2 samples, thereby facilitating the identification of the ferroelectric configuration.

HL 24.10 Wed 12:00 POT/0081

Robust Orbital-Selective Flat Bands in Transition-Metal Oxychlorides — Xiangyu Luo[1], •Ludovica Zullo[2], Sahaj Patel[1], Dongjin Oh[1], Qian Song[1], Asish K. Kundu[3], Anil Rajapitamahuni[3], Elio Vescovo[3], Natalia Olszowska[4], Rafal Kurleto[4], Dawid Wutke[4], Giorgio Sangiovanni[2], and Riccardo Comin[1] — [1]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]Universität Würzburg, 97074 Würzburg, Germany, ct.qmat — [3]National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA — [4]Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland

Flat electronic bands, which amplify electron correlations by quenching kinetic energy, provide an ideal foundation for exotic quantum phases. Here, we unveil an intrinsic orbital-selective flat-band mechanism in the van der Waals materials $NbOCl_2$ and $TaOCl_2$, directly observed by angle-resolved photoemission spectroscopy (ARPES) and understood through density functional theory (DFT) and Wannier analysis. Crucially, we experimentally demonstrate that this momentum-independent flat band exhibits remarkable robustness, surviving from the bulk crystal down to the few-layer limit at room temperature. Our theoretical analysis traces its origin to the hybridization between Nb-dz^2 orbital chains and the Lieb-like dx^2-y^2 sublattice, which is further reinforced by Peierls dimerization. Our findings uncover a new orbital-selective design principle for realizing flat bands in quantum materials.

HL 24.11 Wed 12:15 POT/0081

Tuning the Metal-to-Semiconductor Transition in Bilayer PtTe2 via Electric Field Control — •Sharieh Jamalzadeh Kheirabadi, Farzan Gity, Paul K.Hurley, and Lida Ansari — Tyndall National Institute, University College Cork, Cork, Ireland

Abstract: One effective method to induce a bandgap in graphene is applying a perpendicular electric field to its bilayer structure [1]. This process works by breaking the inversion symmetry of BL gra-phene with an external electric field, leading to electrostatic screening between the two layers and splitting the π and π^* bands that intersect at the Fermi level [2]. Platinum ditelluride (PtTe2) has garnered significant interest due to its unique physical and chemical properties [3,4]. PtTe2 retains its semi-metallic properties for thicknesses down to BL but transits to a semiconductor when re-duced to a monolayer due to the quantum confinement effect [5]. We demonstrate that a bandgap emerges in BL-PtTe2 when an electric field is applied perpendicular to the layers, ultimately trans-forming the system into a semiconductor. We have identified reliable critical electric fields within the range of 2-3 MV/cm to achieve a bandgap comparable to conventional semiconductors in BL-PtTe2. Further, we have investigated the effect of a

vertical electric field on a BL-PtTe2 based field effect transistor using density functional theory (DFT) and non-equilibrium Green*s function (NEGF) methods. The results demonstrate device performance compatible with low-power require-ments for ION and IOFF, as projected in the IRDS 2028 roadmap [6].

HL 24.12 Wed 12:30 POT/0081

Circular Dichroism ARPES Reveals Orbital Chirality in Single-Layer TMDs — •Shubham Patel, Luke Pimlott, and Habib Rostami — Department of Physics, University of Bath, Claverton Down BA2 7AY, United Kingdom

The electron wavefunctions in momentum space are fundamental to understanding the microscopic physical properties of solids. Circular dichroism (CD), a key feature observable in angle-resolved photoemission spectroscopy (ARPES) [1]. Recent experimental investigations have indicated a direct relationship between CD-ARPES and the Berry curvature of electronic bands [2], motivating theoretical efforts to interpret CD within this framework. The Berry curvature-based approach fails to capture certain critical sign-reversal features near the time-reversal-invariant K(K') points. Moreover, this method lacks dependence on the photon energy of the incident light, as it is derived purely from the momentum-space wavefunction characteristics. In the present work, we adopt this plane wave approximation to compute CD-ARPES spectra and find excellent agreement with experimental observations. We solve tight-binding Hamiltonian for single-layer TMDs, and generalize the dipole matrix elements. This formalism successfully captures the sign-changing behavior of CD near the K(K') points, a feature absent in the Berry curvature approach, and provide a control on tunability of the dichroic response with the photon energy. Notably, our theoretical approach offers an alternative explanation that differs from the Berry curvature-based framework.

[1] PRL 110, 216801 (2013) [2] PRL 121, 186401 (2018)

HL 25: 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 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 Rudolf Bratschitsch, Alexander Holleitner, and the AGyouLeaP (Lucas Kreuzer and Aisha Aqeel)

Time: Wednesday 9:30–12:15 Location: POT/0251

Invited Talk HL 25.1 Wed 9:30 POT/0251

Quantum dots for single-electron current sources — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Niels Ubbelohde, Klaus Pierz, Hans W. Schumacher, and Frank Hohls — Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Generating accurate currents can be achieved in an elegant and direct way by applying a periodic signal to a tunable barrier quantum dot. Such devices are called single-electron pumps (SEPs) due to their capability of emitting a well defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e this leads to a controlled and clocked current of $I = nef$, thereby providing a suitable basis for a quantum current standard. While individual SEPs can already achieve errors in the sub-ppm range for currents of the order $I \approx 100$ pA [1], implementing larger systems consisting of multiple well-performing SEPs remains a challenging task. We here present DC transport as well as pumping characteristics of multiple SEP devices toward scaling to higher currents.

[1] F. Stein, et. al., Metrologia 54, S1-S8 (2017)

Invited Talk HL 25.2 Wed 10:00 POT/0251

Optical readout of reconfigurable in-plane magnetic domains in CrSBr — •Aleksandra Łopion[1], Pierre-Maurice Piel[1], Manuel Terbeck[1], Jan-Hendrik Larusch[1], Jakob Henz[1], Marie-Christin Heissenbüttel[2], Thorsten Deilmann[2], Michael Rohlfing[2], Zdenek Sofer[3], and Ursula Wurstbauer[1] — [1]Physikalisches Institut and Center for Soft Nanoscience (SoN), University of Münster, Wilhelm Klemm Str. 10, Münster, 48149, Germany — [2]Institut für Festkörpertheorie, University of Münster, Wilhelm Klemm Str. 10, Münster, 48149, Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague Technická 5, Prague, 616628, Czech Republic

Two-dimensional van der Waals (vdW) magnets have overcome the Mermin-Wagner expectation by hosting long-range order while remaining tunable through stacking, strain, gating, and external fields. Their reconfigurability and hysteresis are attractive for information technologies, particularly when antiferromagnetic (AFM) multistability is accessed and read optically. We discover a reconfigurable multilayer magnetic domain structure in the A-type antiferromagnetic semiconductor. The layered out-of-plane domain structure can be tuned by external stimuli and read out via domain-modulated optical contrast. This coupled magnetic-optical functionality demonstrates the possibility of encoding, processing, and storage of information in magnetic textures with a photonic-compatible readout. The domain landscape highlights CrSBr as a platform for "intelligent matter" and a building block for ultracompact opto-spintronic memories and neuromorphic hardware.

Invited Talk HL 25.3 Wed 10:30 POT/0251

Ferroelectric switching in Mn-doped epitaxial $BaTiO_3$ films and superlattices on silicon — •Alfredo Blázquez Martínez[1], Valentin Väinö Hevelke[1,2], Ibukun Olaniyan[1,2], Minh-Anh Luong[1,3], Ines Häusler[1], Sven Wiesner[1], Christoph T. Koch[4], Dong-Jik Kim[1], and Catherine Dubourdieu[1,2] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie, 14109 Berlin, Germany — [2]Freie Universität Berlin, 14195 Berlin, Germany — [3]CEMES-CNRS and Université de Toulouse, F-31055 Toulouse, France — [4]Humboldt-Universität zu Berlin, 12489 Berlin, Germany

The integration of epitaxial ferroelectric oxides on silicon remains a key challenge for realizing energy-efficient and CMOS-compatible nanoelectronic devices. Among these materials, barium titanate ($BaTiO_3$) is a prototypical perovskite ferroelectric with a high remanent polarization and a low coercive field. Molecular beam epitaxy (MBE) enables the growth of high-quality epitaxial $BaTiO_3$ on Si, yet these films typically show high leakage currents, which preclude polarization measurements and the realization of functional devices on Si. Here, we demonstrate robust ferroelectric hysteresis in epitaxial $BaTiO_3$ films grown on p-type Si using Mn doping. The introduction of a suitable amount of Mn suppresses leakage currents by up to seven orders of magnitude. We will then discuss the properties of (Mn-doped $BaTiO_3/SrTiO_3)_n$ superlattices hosting vortex polar textures of a few nanometers in diameter. This work highlights Mn-doping as an effective path to reduce leakage currents in epitaxial $BaTiO_3$ heterostructures to enable future topotronic devices integrated monolithically on semiconductors.

15 min. break

Invited Talk HL 25.4 Wed 11:15 POT/0251

Tunability of quantized Hall plateaus — •Serkan Sirt[1], Vladimir Umansky[2], and Stefan Ludwig[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Weizmann Institut of Science, Rehovot, Israel

The textbook single-particle description of the quantum Hall effect based on the Landauer-Büttiker picture explains the extent of quantized Hall plateaus as a function of magnetic field in terms of disorder-broadened Landau levels. In contrast, the screening theory includes electron-electron interactions and predicts the formation of extended

Hall plateaus based on the confinement potential, without the need for disorder [1].

To test these contrasting models, we investigate the tunability of the plateaus in gate-defined Hall bars. We employ a global top gate to deplete the two-dimensional electron system and an additional screen gate on the sample surface, separated by an insulating layer, to define the Hall bar. Varying the gate voltages allows us to tune the edges of the Hall bar continuously from hard to soft confinement. We find that, for softer confinement, the plateaus become wider by extending to lower magnetic fields. These results support the screening theory and are inconsistent with the Landauer-Büttiker picture.

This work establishes a new method for controlling and manipulating quantized Hall plateaus, which may become relevant for quantum Hall metrology and quantum technology applications.

[1] R. R. Gerhardts, Phys. Status Solidi B 245, 378 (2008)

Invited Talk HL 25.5 Wed 11:45 POT/0251

How to achieve high gain in organic photodetectors? — •Johannes Benduhn — Institute of Applied Physics, TU Dresden, Germany — German Centre for Astrophysics, Görlitz, Germany

Organic photodetectors (OPDs) match their inorganic counterparts in performance, with additional features like semitransparency, flexibility, and narrowband detection, opening new sensing applications. However, high-gain OPDs are challenging due to disorder. This work discusses two alternative principles to achieve gain.

The first approach uses unbalanced charge-carrier transport. Photogenerated charges accumulated near one of the contacts generate a local field that triggers charge injection of charges from the external circuit into the active layer. Under dark conditions, this injection is absent; therefore, these devices reach impressive EQE values of 1,000-10,000 %. However, the underlying microscopic mechanisms remain unclear. Here, we precisely tune the interface layers via vacuum deposition, enabling us to reveal the injection mechanism.

Another solution is photoactive transistors. We introduce vertical organic-permeable base transistors (OPBTs) that operate at low driving voltages and achieve high switching speeds. We report, for the first time, a photogating effect in OPBTs. By leveraging the unique structure of OPBTs and conducting a detailed investigation into the underlying charge-storing mechanism, we have achieved record responsivity values reaching 10^9 A/W, specific detectivities of 10^{15} Jones (based on noise measurements), and retention times exceeding 10^5 s. [1]

[1] Schröder, Benduhn *et al.* Nature Photonics 19, 1088-1098 (2025).

HL 26: Poster II

Time: Wednesday 9:30–11:30 Location: P1

HL 26.1 Wed 9:30 P1

Quantum Dots in Nonlinear Mechanical Resonators — •Jona Richter, Noah Spitzner, Emeline Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Münster, Germany

Surface acoustic waves are employed in a broad range of technologies, including radio-frequency filters in wireless communication systems and life-science applications. In the presented work, SAWs are utilized to drive mechanical modes in a quantum-dot membrane patterned into rings on a lithium niobate substrate. Generation of the SAWs is achieved by fabricating a comb-shaped interdigital transducer on the substrate. When an RF signal is applied, the piezoelectric response of the lithium niobate converts the electrical excitation into coherent acoustic waves propagating on the surface of the substrate. The propagating SAW induces a periodic modulation of the QD lattice constant, resulting in a corresponding modulation of the emission energy at the driving frequency. This mechanism enables the use of individual QDs as point-like nanoscale sensors, which can be probed through photoluminescence spectroscopy using ultrafast optical detection. When sweeping the RF frequency over a range of 200-900 MHz, pronounced resonances in the emission-energy modulation are observed, but only for QDs located within the ring structures. Both time-integrated as well as time-resolved measurements exhibit clear signatures of nonlinear mechanical behavior for example a hysteresis.

HL 26.2 Wed 9:30 P1

Gallium Nitride arrays for proton imaging — •Nico Frédéric Brosda[1], Matilde Siviero[2], Maxime Hugues[2], Stéphane Higueret[3], Nicolas Arbor[3], Andreas Wieck[1], and Jean-Yves Duboz[2] — [1]Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, D-44780 Bochum, Germany — [2]Université Côte d'Azur, CNRS, CRHEA, 06560, Valbonne, France — [3]Université de Strasbourg, CNRS, IPHC UMR 7178, F-67000 Strasbourg, France

The MATRIX project is advancing proton therapy for cancer treatment by developing novel, highly durable detectors designed to improve real-time control of irradiation doses. Proton detection is performed by measuring the charge generated within the active regions of PIN GaN diodes. These GaN-based devices are fabricated as linear arrays containing 128 diode elements, as well as two-dimensional imaging arrays with up to 11×11 elements, covering an area of 1 cm^2 and achieving spatial resolutions of up to 500 μm. Owing to microelectronic fabrication techniques, even higher resolutions can be realized when required. The spatial performance of these detectors was validated through proton radiography of test objects using a 24 MeV beam, benchmarked against non-pixelated Gafchromic film. Measurements with phantoms of varying thickness further demonstrated the detector's capability for energy-resolved proton imaging. With achieved frame times of 1 ms, the MATRIX detector also provides a first proof of concept for real-time proton beam monitoring.

HL 26.3 Wed 9:30 P1

Impact of Ge-doping on the photoelectrochemical response of cubic (Ga,In)N photoelectrodes — •Sundas Hamid[1,2], Marius Wasem[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

(Ga,In)N is a promising electrode material for electrochemical water splitting as the amount of indium determines the band gap of the semiconductor alloy. In this study we focus on the influence of germanium doping on the photoelectrochemical response of cubic (In,Ga)N photoanodes, which were grown by molecular beam epitaxy (MBE). Different methods like open circuit potential, cyclic voltammetry and electrochemical impedance spectroscopy were used to analyse charge carrier transport and the properties of the electrode electrolyte interface, such as flat band potential. The non-intentionally doped samples show a high photocurrent, indicating less recombination and efficient charge separation, while doping decreases the photoelectrochemical response. Despite the lower photocurrent, the doped samples show higher electrochemical stability displaying structural strength and chemical resistance at the interface. The results show that a trade-off between stability and activity needs to be achieved by controlling doping and indium concentration to develop durable and efficient III-nitride photoanodes for solar water splitting.

HL 26.4 Wed 9:30 P1

First Principle Calculations of Scandium-Aluminium-Nitrides — Max Grossmann, Malte Grunert, and •Wichard beenken — Technische Universität Ilmenau, Institut für Physik, Theoretische Physik I, Ilmenau, Germany

We have calculated the crystal structures and optical spectra of $Sc_xAl_{1-x}N$ compounds in trigonal/hexagonal and tetragonal/cubic lattices. For increasing Scandium content, we could confirm the experimentally found first order phase transition from Wurtzit to Rock-Salt structure. Furthermore we found a second order phase transition to the theoretically predicted metastable hexagonal-MgO-structure. Thereby, we studied various possible superstructures for rational Scandium to Aluminium proportions in detail. Using LDA, *GW*, and BSE methods, we calculated band structures and optical dielectric functions for selected $Sc_xAl_{1-x}N$ compounds with high precision.

HL 26.5 Wed 9:30 P1

Tracing Charge Carrier Transport in Freestanding Core-Shell GaN Nanowires on n-Si(111) Substrates — •Juliane Koch[1], Patrick Häuser[2], Peter Kleinschmidt[1], Lisa Liborius[2], Nils Weimann[2], and Thomas Hannappel[1] — [1]Technische Universität

Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]University of Duisburg-Essen, Components for High Frequency Electronics (BHE) and CENIDE, Duisburg, Germany

Precisely engineered heterojunctions are essential for advancing nanoscale systems with superior electrical performance. The structure and electrical behavior of nanostructured devices must be examined with high spatial resolution. This study investigates the charge carrier transport in freestanding core-shell GaN nanowires (NW) grown via polarity- and site-controlled metal-organic vapor phase epitaxy with a site-dependent AlN interlayer on pre-structured n-type Si(111) substrates. Multi-tip scanning tunnelling microscopy and electron beam-induced current mapping were utilized to probe local transport phenomena with high precision. Transport pathways of charge carriers within the NWs and across key interfaces were resolved. Distinct I-V characteristics appeared for different facets, while scanning transmission electron microscopy revealed no direct shell-core contact. Consequently, current transport is governed by three serially connected diodes: shell-shell, shell-core, and NW-substrate junctions. These results reveal mechanisms shaped by geometry and interfaces, advancing understanding of charge carrier dynamics in III-N nanostructures.

HL 26.6 Wed 9:30 P1

Optical loss characterization in UV multimode AlGaN waveguides with and without a backside absorbing layer — •Leonardo Wildenburg[1], Verena Kowallik[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Photonic integrated circuits (PICs) in the UV range enable complex optical functions on a chip-scale platform, e.g. for the detection of gases and biomolecules by absorption or Raman spectroscopy. The implementation of UV PICs requires wide-bandgap materials to ensure optical transparency. Among the available material systems, one promising candidate is AlGaN due to its application in UV-LEDs and laser diodes. In this work, the optical losses near 265 nm of n-$Al_{0.76}Ga_{0.24}N$ waveguides with a width of 200 μm are investigated using a monolithically integrated UV-LED and UV-photodetector. The influence of straylight from the substrate backside was investigated with and without an absorbing 200 nm thin SiN layer. When operating the LEDs at a constant output power of 0.2 mW, the photocurrent decreases exponentially with increasing waveguide length according to Beer-Lambert-law. The reduction of scattered light was confirmed by measurements of photodetectors of the same wafer, but not connected to the emitting LED by a waveguide. Thus, optical losses of (40 ± 5) cm^{-1} with an absorbing layer and (33 ± 5) cm^{-1} without were measured for the n-$Al_{0.76}Ga_{0.24}N$ waveguides. It was also determined that the optical losses strongly depend on the amount of scattered light from the UV-LED signal.

HL 26.7 Wed 9:30 P1

Optimization of etching processes for quantum well structures to enhance IR emission — •Daniel Janzen[1], Peter Zajac[1], Sascha R. Valentin[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund

The precise control of etching processes is crucial for the properties of quantum well structures, especially in terms of IR emitter efficiency. This study examines how different etching techniques affect surface quality, defect formation, and electrical properties of the epitaxially grown GaSb layers. A critical aspect is the formation of oxides and metallic antimony, which can lead to leakage currents and short circuits. Through Atomic Force Microscopy (AFM) the influence of etching parameters are investigated. Reducing defect states and optimizing material passivation could contribute to the long-term improvement of emission efficiency. This research bridges materials science and semiconductor physics by discussing strategies to optimize surface states for IR emitters. The findings are relevant not only for quantum optics but also for sensor applications and industrial semiconductor fabrication.

HL 26.8 Wed 9:30 P1

Hydrogen Annealing of Silicon Micro- and Nanostructures through Rapid Thermal Processing — •Kyra Malcherek, Thomas Grap, and Markus Kaiser — Helmholtz Nano Facility, Forschungszentrum Jülich, Germany

As semiconductor devices continue to scale into the lower nanometer range, achieving smooth surfaces becomes increasingly important for device performance. In particular, silicon nanowires used in Gate-All-Around Metal-Oxide-Semiconductor Field-Effect Transistors (GAA-MOSFETs) require these characteristics to ensure uniform electrostatic control over the channel. Therefore, Hydrogen Annealing of silicon is a promising process to enable shape transformation and surface smoothing.

In this study, we characterized the effects of Hydrogen Annealing. Silicon microstructures showed a significant reduction in surface roughness and rounded corners after the process. In addition, stable crystal facets were formed and identified as (111) and (113) planes. The influence of the relevant process parameters - temperature, annealing time, hydrogen flow and pressure - were investigated. The radius of curvature increases with both temperature and annealing time, whereas hydrogen flow and pressure show no significant influence.

The process was further applied to silicon-on-insulator nanostructures, creating free-floating silicon nanowires after oxide etching. Subsequent hydrogen annealing effectively smoothed and rounded the structures, demonstrating its potential for the fabrication of GAA-MOSFETs.

HL 26.9 Wed 9:30 P1

Processing and Characterization of Mid Infrared Emitters from III-V Epitaxy — •Peter Zajac[1], Sascha R. Valentin[1], Timo A. Kurschat[1], Rainer Krage[1], Arne Ludwig[2], and Andreas D. Wieck[3] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany — [2]Arbeitsbereich Epitaxie, Experimentalphysik VI, Ruhr-Universität Bochum, 44801 Bochum, Germany — [3]ehem. Lehrstuhl für Angewandte Festköperphysik, Ruhr-Universität Bochum, 44801 Bochum, Germany

A layer structure optimized for mid-infrared emission, containing W-type quantum wells has been realized with III-V epitaxy on GaSb. The processing workflow presented here, from the MBE-grown wafer sample to an emitting device, includes mesa etching, photolithography and electrical contacting. The contribution outlines the challenges faced in progressing towards the first prototype, including the optimization of the wet-etching process with respect to the observed trench formation and surface roughness. The electrical characterization includes contact resistance and I-V measurements. Electroluminescence spectroscopy is performed for optical characterization.

HL 26.10 Wed 9:30 P1

GaAs nanowire networks by electrochemical etching as a universal platform for oxide and nitride architectures — •Eduard Monaico[1], Sebastian Lehmann[2], Elena Monaico[1], Xinzhi Li[2], Veaceslav Ursaki[1], Ion Tiginyanu[1], and Kornelius Nielsch[2] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany

GaAs nanowire networks obtained by electrochemical etching provide a versatile platform for semiconductor-oxide-nitride architectures with controlled geometry and crystallinity. Depending on the orientation of the GaAs substrate ((100), (111)B, (001)), the resulting nanowires can be tilted, vertical, or oriented parallel to the surface. Formed by selective electrochemical dissolution rather than epitaxial growth, they retain the structural quality of the bulk crystal, offering a low-defect scaffold suitable for subsequent transformations.

In this work, we explore their conversion into oxides and nitrides. Thermal treatment in argon with 3% oxygen led to selective formation of Ga2O3 on the nanowires while preserving the GaAs substrate, confirmed by SEM, EDX, XRD, and Raman analysis. Preliminary nitridation tests also show the feasibility of forming GaN-based architectures. These findings highlight the potential of electrochemically derived GaAs nanowire networks as a universal platform for oxide and nitride structures relevant to optoelectronics, photonics, and sensing technologies.

Acknowledgements: We thank the BMFTR and NARD for the funding of ProMoMo project DEHYCONA.

HL 26.11 Wed 9:30 P1

Influence of AlInP(100) Surface Reconstruction on TiO_2/III–V Interface Chemistry and Band Alignment — Mohammad Amin Zare Pour[1,2], Christian Höhn[3], Negin Mogharehabed[1], Roel van de Krol[3], Thomas Hannappel[2], and •Agnieszka Paszuk[1] — [1]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

TiO_2/III–V heterointerfaces are crucial for photoelectrochemical de-

vices, as their chemistry and band alignment govern photogenerated charge-carrier transfer. The TiO_2/InP(100) heterointerface was recently studied using XPS/UPS and *ab initio* molecular dynamics simulations [Adv. Funct. Mater. 2025, 2506105]. ALD-grown TiO_2 on phosphorus-terminated (P-rich) InP(100) shows strong interface-induced band bending, $InPO_x$ formation related to the P-rich surface, and Cl incorporation from $TiCl_4$, reflecting precursor-dependent chemistry. Here, we relate these findings to AlInP(100) surfaces prepared with either P-rich or indium-rich termination, as well as with a thin oxide layer. By comparing oxide states and valence-band positions with those of InP, we analyze how surface reconstruction governs the formation and energetic alignment of TiO_2/III–V heterointerfaces. These insights highlight how AlInP surface preparation controls the formation and electronic structure of TiO_2/III–V interfaces.

HL 26.12 Wed 9:30 P1

Measuring the Temperature Distribution of GaSb Wafers during MBE Growth — •Timo A. Kurschat[1], Sascha R. Valentin[1], Peter Zajac[1], Rainer Krage[1], Arne Ludwig[2], and Andreas D. Wieck[3] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund — [2]Arbeitsbereich Epitaxie, Experimentalphysik VI, Ruhr-Universität Bochum, 44801 Bochum — [3]ehem. Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44801 Bochum

During epitaxial growth the substrate temperature is one of the essential parameters. To obtain high-resolution temperature maps we use a single-lens reflex (SLR) camera with the infrared filter removed. The sensor is sensitive up to a wavelength of about 1 μm and can therefore be used as a pyrometer. With wafer rotation disabled, temperatures down to $T_S = 400\,°C$ can be measured. With rotation and a reduced exposure time of 0.25 s images can still be obtained at the growth temperature of $T_S = 680\,°C$.

To optimize the temperature distribution, so called washers are used during growth that cover parts of the wafer. With the original washers, the center of our quarter 2" wafers is more than 20 K hotter than the corners. Without a washer the profile inverts. Therefore we designed a new washer which greatly improves the homogeneity.

On the other hand an inhomogeneous temperature profile can be used to optimize growth parameters, which we show with photoluminescence measurements of quantum wells and atomic force microscope images.

HL 26.13 Wed 9:30 P1

Impact of Al containing nucleation layers on Si(100)/GaP heterointerface — •Kai Daniel Hanke[1], Angieszka Paszuk[1,2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]Technische Universität Ilmenau, BMFTR Junior Research Group PARASOL, Ilmenau, Germany

Monolithically grown III-V-on-silicon (100) tandem solar cells show great promise for applications such as direct solar water splitting. A critical interface in these devices is the Si/GaP heterointerface, at which defects originate and subsequently propagate through the entire III-V epitaxial stack. Minimizing defect formation at this initial interface is therefore essential for achieving high-efficiency water-splitting performance. The use of TMAl during the pulsed nucleation of the GaP layer has previously been shown to lower defect densities, particularly stacking faults, stacking-fault pyramids (SF/SFP), and threading dislocations (TDs). In this study, we investigate the effect of TMAl on the formation of SF/SFP and on the density of TDs. We further analyze how TMAl modifies the interfacial energetic band alignment using X-ray photoelectron spectroscopy, and study its impact on surface anisotropy and interface-related optical transitions by low-temperature reflection anisotropy spectroscopy. Defect densities are quantified by electron channeling contrast imaging, a scanning electron microscopy technique that exploits electron channeling at an acceleration voltage of 30 kV.

HL 26.14 Wed 9:30 P1

Enhanced Field Emission Current Density in Chemically Engineered Multiwall Carbon Nanotube Neodymium Oxide Heterostructures — •Anima Mahajan[1], Menaka Jha[2], and Santanu Ghosh[1] — [1]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi -110016, India. — [2]Institute of Nano Science & Technology, Knowledge City, Sector-81, Mohali, Punjab-160062, India.

The MWCNT, neodymium oxide (Nd*O*), and MWCNT-Nd*O* heterostructure were successfully fabricated through a facile three-step synthesis process: the synthesis of MWCNT rods by the chemical vapor deposition technique, the synthesis of the Nd*O* nanoparticles by using the micellar-assisted solid-state route, and the fabrication of the MWCNT-Nd*O* heterostructure. Moreover, the MWCNT-Nd*O* heterostructure exhibits enhanced field emission properties, with a lower turn-on field of 2.4 V/*m compared to pure MWCNT and Nd*O*, which have turn-on fields of 3.6 and 3.8 V/*m, respectively. The MWCNT*Nd*O* heterostructure exhibits an enhancement in current density of approximately 6365% compared to pure Nd*O* and around 172% relative to pristine MWCNT. The emission current stability at a preset value of 6 V/*m over an 8-hour duration is found to be fairly good, characterized by current fluctuations within * 3% of the average value. The enhanced field emission (FE) performance of the MWCNT-Nd*O* heterostructure is attributed to its high enhancement factor (β) of ~3.3*10*.

HL 26.15 Wed 9:30 P1

Low temperature photoluminescence excitation spectroscopy on thin film zinc phthalocyanine — •Josephine Braun, Sebastian Hammer, and Jens Pflaum — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The optical properties of molecular semiconductors are determined by the electronic properties of the molecular constituents and their respective inter-molecular (IM) interaction [1]. To disclose the IM interaction, polymorphic materials like Zinc-phthalocyanine (ZnPc) provide perfect prototypical systems [2]. Its luminescence in the α-phase is dominated by excimer emission [3], wheras the β-phase luminescence is governed by a highly temperature sensitive Frenkel exciton emission. While temperature dependent luminescence studies provide insight into the IM interaction potential, the excitation spectrum does the same without being prone to effects of excitonic relaxation. In this contribution we investigate the excitonic system of ZnPc thin films in the α- and β-phase via temperature dependent photoluminescence excitation (PLE) and photoluminescence (PL) spectroscopy between 4 K and 300 K. We show, that while the PL spectra exhibits strong variability with temperature, the PLE spectra show only minor changes. This suggests that rather than a large modulation of the IM interaction with temperature, exitonic relaxation processes are at the heart of ZnPc's pronounced spectral luminescence changes.

[1] Hestand and Spano, *Chem. Rev.* **118** (2018), p. 7069–7163
[2] Hammer et al., *Appl. Phys. Lett.* **115** (2019), p. 263303
[3] Hammer et al., *Mater. Horiz.* **10** (2023), p. 221–234

HL 26.16 Wed 9:30 P1

Host-Emitter Interactions in Single-Gaussian Deep-Blue Europium(II) OLED Emitters — •Mahmoud Soleimani[1,2], Paulius Imbrasas[2], Jan-Michael Mewes[2], Felix Kaden[2], Sebastian Schellhammer[1], Toni Bärschneider[2], Carsten Rothe[2], and Sebastian Reineke[1] — [1]Institute of Applied Physics (IAP), Technische Universität Dresden, Germany — [2]beeOLED GmbH, Dresden, Germany

Lanthanide-based emitters offer a promising approach to stable and efficient deep-blue organic light-emitting diodes (OLEDs). While divalent europium [Eu(II)] and trivalent cerium [Ce(III)] can provide ideal emission colors with near-unity exciton utilization, their integration into thin-film architectures remains insufficiently understood. In particular, the compatibility of lanthanide complexes with organic host materials and possible lanthanide-specific interactions are open questions. To shed light on and gain a deeper understanding of these aspects, we combine photoluminescence spectroscopy and density functional theory to evaluate the behavior of a literature-reported Eu(II) emitter and to introduce two new carborate-based Eu(II) complexes. These novel materials exhibit deep-blue single-Gaussian 4f-5d emission. Our experimental and theoretical analysis provides a framework for understanding electron confinement and shielding in Eu-based emitters, establishing design principles for a new class of stable, efficient deep-blue OLED materials.

HL 26.17 Wed 9:30 P1

Flexible OLED-OPD System in a Rolled Geometry for Angle-Resolved Optical Sensing — •Shujun Pei, Jan Schardt, Markus Köpke, and Martina Gerken — Chair for Integrated Systems and Photonics, Faculty of Engineering, Kiel University, Kiel, Germany

We investigate an integrated sensing platform combining an organic light-emitting diode (OLED) and multiple organic photodetector

(OPD) pixels fabricated on a single flexible PET substrate. After fabrication, the substrate is rolled manually such that the OLED and OPDs face each other across the inner circumference of a cylindrical channel. This geometry enables angle-dependent optical paths through fluids flowing inside the tube, providing a basis for reconstructing absorption and scattering profiles relevant for chemical and biomedical sensing.

To independently assess OLED-OPD performance, devices were characterized on separate flat substrates. OPD responsivity was quantified using a calibrated LED solar simulator and direct OLED illumination. Distance-dependent photocurrent measurements reveal the expected decay consistent with Lambertian emission and simple geometric coupling between the OLED and OPD pixels. Numerical modeling, including finite emitter and detector areas as well as realistic alignment offsets, closely reproduces the measured photocurrent trends.

These results demonstrate the feasibility of compact, flexible OLED-OPD assemblies for multi-angle optical sensing and provide a foundation for future device refinement.

HL 26.18 Wed 9:30 P1

Organic Narrowband Near-infrared Photodiodes for Breath Monitoring — •Sudhi Mahadevan[1,2], Siddhartha Saggar[1,2], Rabiul Islam[1,2], and Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, Kurt-Schwabe-Straße 4, 04736 Waldheim, Germany

For clinical diagnosis of various diseases, breath analysis has become a powerful non-invasive tool, which demands the development of reliable and efficient sensing technologies. However, conventional respiratory monitors hinder users' mobility, provide discomfort, and affect natural breathing patterns. Recent progress in organic and wearable optoelectronics presents an opportunity to develop thin, flexible, and imperceptible sensors. In this work, we report high-performance near-infrared (NIR) organic photodiodes (OPD), using a PM6:Y6 blend combining a polymer donor with an NIR-absorbing small molecule processed from the green solvent o-xylene. In this simplified device architecture, the hole-blocking functionality is incorporated directly into the active layer, reducing fabrication complexity and enabling cost-effective production. A narrow-band optical response at 800 nm is achieved via an organic photo-filtering layer that allows only long-wavelength photons into the active layer. The optical breath sensor will integrate organic light-emitting diodes (OLEDs) to emit light onto the chest, while an OPD will capture changes in diffusely scattered light from the skin during breathing. This work aims to advance organic electronic devices into the NIR spectrum for non-invasive medical diagnosis applications.

HL 26.19 Wed 9:30 P1

Wavelength-selective, ultraviolet (Mg,Zn)O photodiodes — •Jonas Elz, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Ninety-five percent of the UV radiation that reaches the Earth's surface is in the UVA band (315-400 nm). In order to assess the potential harmful effects of UVA radiation on the human epidermis with compact, wearable devices, semiconductor technology can be used. Magnesium zinc oxide is a suitable material for detectors in such devices because it exhibits a bandgap between 3.3 and 4.8 eV. One photodiode design uses a filter and an active layer with different material compositions to achieve sensitivity in different optical bands [2].

In this study, we use combinatorial pulsed laser deposition to fabricate metal-semiconductor-metal photodiodes that are sensitive to different wavelength ranges. With the same mask system and similar targets as in [3], we achieve multiple compositions of filter and active layers on a single substrate.

[1] von Wenkstern et al. "The (Mg, Zn)O Alloy" in "Handbook of zinc oxide and related materials" pp 257-320
[2] Zhang et al. Appl. Phys. Lett. 108, 243503 (2016)
[3] Thyen et al. J. Vac. Sci. Technol. A 41, 020801 (2023)

HL 26.20 Wed 9:30 P1

Determination of activation energies in vertical co-doped κ-Ga_2O_3 Schottky barrier diodes — •Elise Morawe, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik Halbleiterphysik, Leipzig, Germany

The predicted spontaneous polarization of κ-Ga_2O_3 renders this polymorph of Ga_2O_3 highly interesting for, e.g., high electron mobility transistor devices [1]. As shown by Kneiß et al., vertical Schottky barrier diodes can be realized on pulsed laser deposition (PLD) grown κ-Ga_2O_3 thin films [2]. For that, the addition of tin in the process is mandatory to induce the surfactant-mediated growth of the κ phase [3]. We present κ-Ga_2O_3 thin films grown by PLD on indium tin oxide (ITO) layer on different substrates: c-sapphire and yttria-stabilized zirconia (YSZ). We discuss the influence of co-doping of the κ-Ga_2O_3 thin films with ZrO_2 or SiO_2 in addition to SnO_2 on the performance of Schottky barrier diodes. Furthermore, the activation energies of Sn, Zr and Si in the κ-Ga_2O_3 are determined by thermal admittance spectroscopy.

[1] Juyeong Kim et al, Appl. Phys. Express, 11, 061101 (2018)
[2] M. Kneiß et al, J. Appl. Phys. 130, 084502 (2021)
[3] M. Kneiß et al, APL Mater. 7, 022516 (2019)

HL 26.21 Wed 9:30 P1

How To Tame Your Iodine in Reactive Sputtering and Similar UHV Thin Film Deposition Processes — •Christiane Dethloff, Sebastian Köpp, Sofie Vogt, Lukas Trefflich, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institute for Solid State Physics, Universität Leipzig, Germany

Sputtering in reactive atmospheres involves several challenging conditions, like target poisoning, or a hysteresis of the reactive gas partial pressure, leading to an unstable operation regime [1]. In order to investigate and control these process conditions, and therefore tune the properties of the resulting thin film, a controlled flux of the reactive species is crucial. Commonly, this is achieved by mass flow controllers, when O and N are the reactive gases [2]. However, in the case of an iodine enriched atmosphere this is hardly feasible, due to the corrosive effect and low inlet pressures.

We present an optical measurement setup, enabling real-time measurements of the iodine content in an iodine enriched Ar flow from an iodine vaporizer into a deposition chamber. Our investigations comprise the growth and characterization of functional p-type copper iodide (CuI) thin films by reactive magnetron sputtering under a well defined iodine flux.

[1] D. Güttler *et al.*, Applied Physics Letters 85.25 (2004): 6134 − 6136 DOI:10.1063/1.1835002.
[2] A. Welk, M. Grundmann *et al.*, Physical Review Applied 17.2 (2022): 024007 DOI: 10.1103/PhysRevApplied.17.024007

HL 26.22 Wed 9:30 P1

Investigation of vertical α-Ga_2O_3/$(Al_xGa_{1-x})_2O_3$ diodes grown by pulsed laser deposition — •Veronika Lunova, Sofie Vogt, Paul Bokemeyer, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

With a bandgap of 5.3 eV and a dielectric breakdown field of 10 MV/cm, α-phase gallium oxide is a promising ultra-wide bandgap semiconductor for high-power electronics [1]. Furthermore, alloying with isostructural α-Al_2O_3 is possible without a miscibility gap and allows for even higher band gaps and electrical breakdown fields [2]. In this work, we present a systematic investigation of vertical Schottky diode structures based on α-$(Al_xGa_{1-x})_2O_3$ thin films grown by pulsed laser deposition (PLD). The heterostructures consist of an undoped α-Ga_2O_3 buffer layer, highly doped intermediate layers, and an $(Al_xGa_{1-x})_2O_3$ layer. Achieving sufficient conductivity in $(Al_xGa_{1-x})_2O_3$ remains a major challenge; thus, we investigate donor activation as a function of aluminum content [3]. The structural quality and electrical properties of the resulting heterostructures were investigated, with focus on the influence of Al incorporation on crystal structure, carrier activation, and vertical transport behavior.

[1] Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).
[2] Hassa *et al.*, J. Phys. D: Appl. Phys. **54** 223001 (2021).
[3] Varley *et al.*, Appl. Phys. Lett. **120**, 262104 (2022).

HL 26.23 Wed 9:30 P1

Titania-based aerodynamic nanomaterials produced by atomic layer deposition — •Tudor Braniste[1], Vladimir Ciobanu[1], Sebastian Lehmann[2], Phil Goldberg[2], Kornelius Nielsch[2], Niklas Wolff[3], Lorenz Kienle[3], Rainer Adelung[3], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute for Solid State and Materials Research, Dresden — [3]Institute for Materials Science, Kiel University, Germany

In this work, we report on a technology for the production of TiO2, Zn2TiO4, and Mg2TiO4 aero-nanomaterials. Titanium and magne-

sium oxides were deposited using atomic layer deposition (ALD) onto a sacrificial network of ZnO microtetrapods. After deposition, the sacrificial ZnO layer was removed using two different technological routes. The first route involves removing the zinc oxide in a citric acid solution at room temperature, followed by critical-point drying of the titania-based material. The second route consists of removing the ZnO substrate in a hydrogen atmosphere at high temperature. At temperatures as high as 850 °C in an atmosphere of H2 + Ar (2% + 98%), the ZnO core decomposes, and the resulting aero-nanomaterial consists of hollow microtetrapods with porous microtubular arms composed of Zn2TiO4 or (ZnMg)TiO2. Scanning and transmission electron microscopy, as well as X-ray analysis, were used to elucidate the morphology, composition, and crystal structure of the produced aeromaterials. The investigations revealed the influence of annealing temperature and the sequence of technological steps on the morphology and properties of the resulting materials.

HL 26.24 Wed 9:30 P1

Band-Gap Trends in Halide Double Perovskites from Quasiparticle Self-Consistent GW — •Louis Meier[1], Timur Biktagirov[1], Volodymyr Vasylkovskyi[2], Anastasiia Kultaeva[2], and Wolf Gero Schmidt[1] — [1]Physics Department, Paderborn University, 33098 Paderborn, Germany — [2]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Halide double perovskites represent a chemically versatile class of optoelectronic materials with tunable band gaps dependent on their cation and halide composition. Their diversity requires a first-principles framework that can predict these trends consistently. Semilocal density functional theory (DFT) underestimates band gaps, while many-body GW results depend sensitively on the DFT starting point. In this contribution, we assess the quasiparticle self-consistent GW (QSGW) method as a unified, starting-point-independent approach for predicting the electronic structure of the $Cs_2MM'X_6$ family (M = Bi, Tl; M' = Ag, Cu; X = Cl, Br), focusing on trends with composition and spin-orbit coupling.

HL 26.25 Wed 9:30 P1

Atomistic Modeling of A- and X-Site Mixing in Halide Perovskites using Cluster Expansion — •Hilde Bellersen[1], Ana M. Valencia[2], and Caterina Cocchi[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Carl von Ossietzky Universität Oldenburg, Germany

Designing stable and efficient halide perovskites involves navigating a vast space of possible chemical substitutions. To address this challenge, we combine density-functional theory calculations with a machine-learning-based cluster expansion framework [1] to efficiently explore multi-component perovskite alloys. Our training structures systematically sample A-site mixing (FA, MA, Cs), X-site mixing (I, Br, Cl), as well as simultaneous A- and X-site co-mixing, with the lattice parameters adjusted according to Vegard's law. These configurations provide the basis for constructing cluster expansion models capable of capturing key energetic trends across the full compositional space. Such models can be used to identify stability landscapes and quantify the influence of configurational effects. We present the methodology, dataset construction, and first insights from the ongoing model development, highlighting the importance appropriate settings to ensure model accuracy, as well as the potential of this approach to guide the design of complex halide perovskite alloys.

[1] M. Ångqvist et al., Advcd Theory and Sims 2, (2019).

HL 26.26 Wed 9:30 P1

Cavity-enhanced microscopy: absorption measurements of single perovskite nanocubes and photo-switchable lipids — •Ayesha Khan[1], Ines Amersdorffer[1,2], David Hunger[3], and Thomas Hümmer[1,2] — [1]Qlibri GmbH, Munich, Germany — [2]Ludwig Maximilian University of Munich, Munich, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Optical studies of nano-scale systems through spectroscopy and imaging can reveal intrinsic optical properties of materials including resolving the exitonic fine structure of systems. However, due to diminutive absorption of nano-scale systems, it is challenging to perform absorption spectroscopy.

For a nano-scale system placed inside an optical resonator, the light passes through the sample thousands of times, enhancing the absorption and thus, allowing measurements.

Here we demonstrate the use of a fiber-based, open-access microcavity to perform direct measurements of the absorption of single perovskite nanocubes. We further image and obtain hyperspectral maps of perovskite nanocubes.

We also present the use of the cavity microscope to image label-free Azo-PC phospholipid bilayers in both cis and trans state and show the diffusion of the two states.

The successful measurements of different nano-scale systems promise that fiber-based microcavities can become standard tools for absorption measurements of these systems.

HL 26.27 Wed 9:30 P1

Excitonic Reststrahlen Effect in $(PEA)_2PbI_4$ — •Michael Pfeufer, Patrick Grenzer, Friedrich Schöppler, and Tobias Hertel — Institute of Physical and Theoretical Chemistry, Julius-Maximilains-University Würzburg, Germany

Layered Ruddlesden-Popper perovskites with their natural quantum well structure allow for strongly confined excitons with very high oscillator strengths. In this work, evidence of an excitonic Reststrahlen effect, a phenomenon in which strong exciton resonances push the real permittivity below zero, was identified and characterized in phenethylammonium lead iodide $(PEA)_2PbI_4$. Transfer-matrix method simulations of the thin film were employed to fit temperature-dependent transmission measurements to an isotropic Lorentz oscillator model and to extract the dielectric function of the material. Additionally, we show that the behaviour of the Reststrahlen band in thickness-dependent transmission spectra is consistent with that found in other materials featuring a Reststrahlen-like response. Electric field calculations inside the material slab suggest natural exciton-polaritonic formation in the material, as well as longitudinal modes near the zero crossing of the real permittivity.

HL 26.28 Wed 9:30 P1

Optical Composition-Property Relationships in a Lead-Free Isostructural 2D Hybrid Metal-Halide Series — •Nils Kasten[1], Jan-H. Littmann[1], Meng Yang[2], Natalie Dehnhardt-Fehst[2], Lukas Gümbel[1], Ralph Kusche[2,3], Markus Stein[1], Johanna Heine[2,3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany. — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, 35043 Marburg, Germany. — [3]Insitute of Chemistry, Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, 26129 Oldenburg, Germany.

Organic–inorganic metal halides have achieved notable success in photovoltaics. Among these, metal-halide perovskites represent a versatile class of compounds, exhibiting diverse optoelectronic behaviour, ranging from narrow-band emission to broadband white-light photoluminescence (PL), typically arising from self-trapped excitons (STEs). These characteristics render them relevant for optoelectronic applications. In this study, we investigate a lead-free isostructural series of two-dimensional hybrid metal halides, $[(R)\text{-1-(4-F)PEA}]_4\,[E_2X_{10}]$; (R)-1-(4-F)PEA = (R)-1-(4-fluoro) phenylethylammonium, where E = Sb, Bi and X = Cl, Br, I. All compounds share a common structural framework, which allows us to isolate the effects of metal-cation and halide-anion substitution on the optical response. We employ PL and Raman spectroscopy to characterize these compounds.

HL 26.29 Wed 9:30 P1

Stokes, Anti-Stokes and selective excitation of Si-vacancies in SiC — •Emilian Eisermann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Our group has demonstrated a room temperature continuous-wave maser that uses the silicon vacancy (V2) in silicon carbide (4H-SiC) (arXiv:2312.08251). Stimulated emission arises from an optically pumped population inversion in these spin defects. However, only a low output power could be achieved and laser heating caused instabilities. To enhance the maser characteristics, we investigate the fundamental pumping behavior of V2 (zero phonon line at 916.2 nm). Hereby, we distinguish between common Stokes excitation (CSE) (<916.2 nm), Anti-Stokes excitation (ASE) (>916.2 nm) and selective excitation (=916.2 nm). Using electron paramagnetic resonance spectroscopy, we resolve microwave absorption and emission signals due to the optical polarization of Zeeman split states. By analyzing these features, we calculate the population inversion and hence the pump efficiency. At low temperatures selective excitation is particular efficient and CSE outcompetes ASE, which requires thermally driven phonons. At room

temperature, the increased phonon activity and the shortened T_1 lifetime cause ASE (λ=950 nm) to have an efficiency of around 50 % compared to CSE. ASE however allows for a very targeted excitation of V2 and we identify an optical pumping sweet spot that is promising for future maser implementations.

HL 26.30 Wed 9:30 P1

Double Gaussian Defect Cavity Design for Semiconductor Based Entangled Photon Sources — •Xian Zheng, Fei Ding, and MIchael Zopf — Institute of Solid State Physics, Leibniz University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Polarization-entangled photon pairs are essential resources for quantum communication and quantum networks, enabling protocols such as quantum key distribution, teleportation, and entanglement swapping. However, simultaneously controlling cavity spectrum, field profile, and balanced coupling to multiple radiative transitions in a solid-state emitter remains challenging. In this work, we design a double-Gaussian defect cavity as a flexible platform to engineer semiconductor quantum-dot entangled photon sources. Two Gaussian-shaped, microsphere-like thickness modulations are embedded inside a DBR cavity and sculpt the axial and lateral field distributions, providing independent knobs, such as cavity height and defect width, to simultaneously tune the cavity resonance close to emission lines, such as biexciton and exciton emission and optimize the emission wavelength. Using FDTD simulations and time-domain exponential decay fitting, we extract the quality factor, mode volume, and Purcell enhancement, and quantify their dependence on the geometric parameters. The resulting design framework provides practical guidelines for tailoring cavity*quantum-dot coupling in double-Gaussian defect geometries and supports the development of bright, on-demand entangled photon sources suitable for future integrated quantum-network architectures.

HL 26.31 Wed 9:30 P1

Low-density InAs quantum dots for telecom O-band single-photon emission — •Elias Kersting, Nikolai Spitzer, Hans Georg Babin, Severin Krüger, Phil Julien Badura, and Arne Ludwig — Ruhr-Universität Bochum, EP6 , Bochum, Germany

InAs quantum dots (QDs) grown by molecular beam epitaxy (MBE) are promising candidates for single-photon sources (SPS), particularly for quantum communication. Emission in the telecom O-band (1260 - 1360 nm) is especially desirable due to the low transmission loss in optical fibers. However, conventional Stranski-Krastanov (SK) InAs QDs face challenges in achieving low and well-controlled densities in the range of 0.1- 10 QDs/um^2, as well as in precisely tuning the emission wavelength. We present an alternative approach to address this issue based on local droplet etching (LDE), in which nanoholes in a GaAs matrix are filled with InAs to form QDs. The quantum dot density is defined by the nanohole pattern, enabling precise and scalable control. A strain-reducing layer (SRL) shifts the emission wavelength into the telecom O-band. Homogeneous low-density (~2 QDs/um^2) growth is achieved through shutter-synchronized deposition, making this approach well suited for scalable SPS fabrication. We detail the fabrication method and present structural and optical characterization results.

HL 26.32 Wed 9:30 P1

Effect of TiO_2 thin films on shallow NV centers in co-doped diamond. — •Arthur Witte, Dominic Reinhardt, Peter Schlupp, Holger von Wenckstern, Jan Meijer, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute for Solid State Physics, Germany

The nitrogen vacancy (NV) center is a color center in diamond, that was proposed as a platform for solid state quantum computing. Essential for this idea is the spin-dependent photoluminescence of the negatively charged NV center, through which an optical spin polarization can be achieved and its relatively long spin coherence time at room temperature. Much research has been done in this direction: to engineer the required negative charge of the NV centers, co-doping of the diamond with donors was developed [1]. Shallow NV centers are subject to surface effects that cause charge instabilities, as well as magnetic and electronic noise. Various surface treatments have been explored to mitigate these effects, including the deposition of a passivation layer on the diamond surface. We combine surface engineering and charge engineering by co-doping and study the effects of these methods on the charge state and T_2 time of shallow NV centers. This is done by sputtering transparent titanium dioxide layers of varying thickness onto a diamond with shallow NV centers in differently co-doped environments. Additionally, effects of annealing of the layer on both the layer itself and the NV properties are discussed.

[1] T. Lühmann, et al. *Phys. Status Solidi a* **8**(1), 1671-1703. (2021)

HL 26.33 Wed 9:30 P1

High-Resolution Lift-Off Process for Sub-100-nm Metal Features using a PMMA Bilayer Stack — •Melina Sporkett[1], Lina Trippelsdorf[1,2], Thomas Grap[1], Florian Lentz[1], and Markus Kaiser[1] — [1]Helmholtz Nano Facility, Forschungszentrum Jülich, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Germany

A reliable and reproducible lift-off process is essential for the fabrication of high-resolution metal structures in micro- and nanotechnology. This has become increasingly important due to recent advances in quantum computing. In quantum devices, these nanoscale electrodes and interconnects are needed to realize the electrical connections to qubits.

In this study, we present a PMMA bilayer lift-off process that enables the reliable fabrication of structures below 100 nm, including fine lines and spaces. The resist stack consists of a copolymer bottom layer that creates a defined undercut and a thin PMMA/CSAR top layer. Through specifically optimized electron-beam lithography and development using a methoxypropanol-based developer, a clearly defined resist profile was achieved. Subsequent metal deposition using Ti/Au electron beam evaporation enabled the fabrication of lines with a width of only 30 nm.

These results demonstrate a robust and practical process for fabricating ultra-fine metallic interconnects for nanoelectronic applications.

HL 26.34 Wed 9:30 P1

Diamond devices for high contrast electrical readout of NV centers — •Melina F. V. Pees[1], Lina M. Todenhagen[1], Joachim P. Leibold[2], Dominik B. Bucher[2], and Martin S. Brandt[1] — [1]Walter Schottky Institut, TU Munich, Am Coulombwall 4, 85748 Garching — [2]Department of Chemistry, TU Munich, Lichtenbergstr. 4, 85748 Garching

Nitrogen-vacancy (NV^-) centers in diamond enable optically and electrically detected magnetic resonance (ODMR and EDMR/PDMR, respectively) and are a promising semiconductor platform for spin-based sensing. Metal contacts often influence the NV^- charge state, change current flow near the surface and worsen the spin contrast in resonance measurements. In this work we investigate shallow, implanted NV ensembles under Ti/Pt/Au contacts using combined photoluminescence, photocurrent and ODMR/EDMR measurements as a function of applied bias voltage, nitrogen implantation depth and position relative to the metallized surface. We have recently shown that Pt, just as other metals, strongly influences the charge state of the NV centers underneath the contacts, leading to mostly neutral or positively charged centers. Here, we show that via application of bias voltages, the negative charge state can be partially recovered, leading to an increase in the spin contrast. This approach allows to stabilize the NV^- charge state and improves the suitability of such diamond devices for quantum sensing applications.

HL 26.35 Wed 9:30 P1

Fabrication of SNSPDs on TF-LNoI for measurement device independent QKD — •Simon Palitza[1,2,3], Bilal Malik[1,2,3], and Carsten Schuck[1,2,3] — [1]Department for Quantum Technology, University of Münster — [2]Center for NanoTechnology - CeNTech, Münster — [3]Center for Soft Nanoscience - SoN, Münster

Thin-Film Lithium Niobate on Insulator (TF-LNoI) has been recognized as a promising platform for realizing low-loss propagation and high-speed modulation of optical signals in photonic integrated circuits. However, quantum technology applications, such as quantum key distribution (QKD) also require integrating single photon detection capabilities with nanophotonic functionalities. Here we show how crucial optical circuit components of a QKD-receiver can be co-integrated with Nb-based Superconducting Nanowire Single Photon Detectors (SNSPDs) on the TF-LNoI-platform. We specifically assess the influence of ubiquitous lithium diffusion on SNSPD performance and explore mitigation strategies in the design and nanofabrication process flow, such as introducing diffusion barrier layers. Combining efficient measurement capabilities with the stability and low loss routing of optical signals in monolithic LNoI-circuits provides a viable way towards realizing quantum communication protocols, such as measurement device independent QKD.

HL 26.36 Wed 9:30 P1

Role of a Quarter-Wave Plate in Resonant Laser Spectroscopy: Signature of Spin-Orbit Interactions of Light — •Wenze Lan, Anton Lögl, and Bernhard Urbaszek — Institute for Condensed Matter Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Resonant laser spectroscopy is a powerful technique for probing the intrinsic optical transitions, coherence properties, and spin dynamics of single quantum emitters. Although polarization-based dark-field confocal microscopy enables nearly background-free detection of resonant fluorescence [1], the role of an additional quarter-wave plate in further improving extinction has remained unclear. Here, we elucidate the mechanism by which a commercial quarter-wave plate enhances polarization extinction in a simple confocal geometry. Under cross-polarization conditions, the transmitted beam exhibits a robust first-order Hermite-Gaussian mode, which explains the improved background suppression and we identify it as a direct signature of spin-orbit interactions of light [2-3]. Our findings inspire applications in polarization optics, nanophotonics, and quantum photonics. [1] Rev. Sci. Instrum. 84, 073905 (2013); [2] J. Opt. 15, 014001 (2013); [3] Nat. Photon. 9, 796-808 (2015).

HL 26.37 Wed 9:30 P1

Phonon-Polaritons in MOVPE-grown hexagonal Boron Nitride — •Oskar Schröer[1], Maximilian Scharpey[1], Lena Miler[2], Johannes Binder[2], Andrzej Wysmołek[2], Daniel Wigger[3], and Iris Niehues[1] — [1]Institute of Physics, University of Münster, Germany — [2]Faculty of Physics, University of Warsaw, Poland — [3]Department of Physics, University of Münster, Germany

Two-dimensional materials composed of atomically thin layers have attracted great interest due to their unique optical and electronic properties. Using a scattering-type scanning near-field optical microscope (s-SNOM), surface phonon polaritons (SPhPs) are observable in the insulating polar van-der-Waals material hexagonal boron nitride (hBN) [1]. While most works focus on exfoliated single-crystalline layers of hBN, we show that SPhPs can also be excited in hBN grown by metalorganic vapor phase epitaxy (MOVPE). Here, grain boundaries and defects play a major role for the propagation properties of the polaritons. By evaluating the real-space interference patterns, we extract dispersion relations and compare propagation characteristics for the two sample types. The results contribute to a deeper understanding of light-matter interactions in polar van der Waals materials and may pave the way towards improved control and manipulation of light-matter excitations on the nanometer scale.

[1] Caldwell et al., Nat. Commun. **5**, 5221 (2014).

HL 26.38 Wed 9:30 P1

Predicting nonlinear optical properties from the linear response: Generalized Miller Formulae — •Maximilian Tim Meyer and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Predicting the nonlinear optical response of real materials from first principles remains a major challenge, since quantitative calculations require strong simplifications and large computational resources. As a shortcut, Miller's rule provides an empirical relation between the linear and second-harmonic coefficients. It can be extended to higher-order nonlinearities and is now accepted as a useful tool for guiding experiments and computational materials discovery. However, its theoretical foundation had long been limited to a simple derivation for the classical Lorentz model with a weak anharmonic perturbation, whose properties differ from those of real quantum-mechanical electrons. We have developed a mathematical framework which enabled us to prove that Miller's rule is nevertheless equally valid for weakly anharmonic quantum-mechanical oscillators [1]. For three-dimensional anharmonic oscillators, we further derived generalized Miller formulae that express all orders of the nonlinear response to an arbitrary multi-frequency field exactly in terms of the linear optical susceptibility [2]. These generalized formulae are applicable to a much broader range of nonlinear optical processes and systems. The practical implementation is illustrated by means of a numerical example. [1] Meyer and Schindlmayr, J. Phys. B **57**, 095001 (2024). [2] Meyer and Schindlmayr, Dynamics **5**, 34 (2025).

HL 26.39 Wed 9:30 P1

Revisiting Cross-Polarized Resonant Excitation: Spin-Orbit Interaction in Confocal Dark-Field Microscopy — •Anton Lögl, Wenze Lan, and Bernhard Urbaszek — Institute for Condensed Matter Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Resonant excitation is a key experiment for accessing and probing the optical properties of semiconductor quantum emitters. The typical epi-fluorescence geometry of the cryostat environment presents an experimental challenge: separating the much weaker emission of the sample from the much stronger excitation, typically addressed using a cross-polarization scheme [1]. It is well known that confocal microscopy in combination with a dark-field technique can surpass the intrinsic extinction limit of commercial polarizers [1, 2]. In this work, we investigate the spin-orbit interaction of light observed when a polarized Gaussian beam is reflected from a mirror surface within such a microscope arrangement. We revisit the model from [2] and demonstrate that slight modifications allow us to phenomenologically model all of our results within the linear and circular polarization basis. Our results pave the way for improved characterization and optimization of optical setups used to measure the optical properties of various quantum emitters. Simultaneously, our results highlight how poorly understood the physical principles of one of the most common characterization techniques in resonant spectroscopy are.

[1] A. V. Kuhlmann, et al. Rev. Sci. Instrum. 84, 073905 (2013)
[2] Benelajla, M. et al. Phys. Rev. X 11, 021007 (2021)

HL 26.40 Wed 9:30 P1

Optical properties of $(Ti_xGa_{1-x})_2O_3$ — •Leonard Käferstein, Clemens Petersen, Daniel Splith, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

The high bandgap energy in the order of 5.3 eV and its high predicted electrical breakdown field of about 10 MV cm^{-1} make α-Ga_2O_3 a quite promising material for transparent electronic devices and high power applications [1]. Alloying αGa_2O_3 with Ti leads to a decrease of the band gap. Here we report on the optical properties, especially the dielectric function, of $(Ti_xGa_{1-x})_2O_3$ determined by spectroscopic ellipsometry as a function of the cation composition.

A $(Ti_xGa_{1-x})_2O_3$ thin film with a lateral composition gradient was deposited by combinatorial pulsed laser deposition [2]. X-ray diffraction indicates a transformation from the tetragonal rutile phase for large Ti concentration ($x > 0.55$) toward a rhombohedral phase for $x < 0.4$. As $(Ti_xGa_{1-x})_2O_3$ is optically uniaxial and the optic axis is within the surface plane, generalized spectroscopic ellipsometry was applied. In the transparent spectral range, we determined a decrease from positive birefringence for high x towards negative birefringence for $x \approx 0$. As expected, we observe a redshift of the bandgap energy with increasing Ti-content from 5.1 eV for $x \approx 0$ down to 4.3 eV for $x \approx 0.85$.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).
[2] H. v. Wenckstern *et al.*, Ph. Status Solidi B **257**, 1900626 (2020).

HL 26.41 Wed 9:30 P1

In situ investigation of PEC devices by time-resolved photoluminescence — •Peter Kleinschmidt, Ali Omar, Sahar Shekarabi, David Ostheimer, and Thomas Hannappel — TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials, 98693 Ilmenau

Direct, unassisted photoelectrochemical (PEC) water splitting is a promising approach for the generation of solar hydrogen. At present, PEC devices still suffer from rapid degradation during operation in the electrolyte. In PEC devices, the control of the dynamics of minority charge carriers is crucial for efficient operation. *In situ* time-resolved photoluminescence (TRPL) measurement provides a direct access to charge carrier lifetimes in the PEC environment. We demonstrate that *in situ* TRPL reveals early-stage, localized degradation in PEC devices under operating conditions long before any decline in conventional performance metrics, such as a reduction in hydrogen evolution current density, becomes detectable. With this method, we investigate the effect of different surface treatments of dual junction PEC devices, in particular the functionalization with passivation layers and catalysts, on the stability and overall performance.

HL 26.42 Wed 9:30 P1

Propagation of Bloch surface polaritons in ZnO — Sebastian Henn, •Dmitry Sayenko, Marius Grundmann, and Chris Sturm — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

Here we present the long-range propagation of Bloch surface polaritons (BSP) in ZnO, which are formed through the strong interaction between light and excitons. Of special interest are BSP particles as they are bosonic quasi-particles and inherit the long-range propagating properties of the involved photons. In contrast to typically used microcavities, BSPs are formed at the surface of a photonic crystal, and thus the fabrication of these structures requires less technical effort and the properties of the BSP are surface-sensitive. In our studies, we realized BSPs in a photonic crystal made of distributed Bragg reflector made of yttria-stabilized zirconia (YSZ) and Al_2O_3. As an active medium, we used a ZnO surface layer, allowing strong coupling up to 430 K [1]. For the coupling of the BSPs to the vacuum modes, a 1D grating was etched onto the surface. By employing non-resonant excitation and varying the distance of the excitation with respect to the grating, the propagation length of BSPs was determined. We found that the propagation length of the BSP is about five times larger than would be expected for a pure photonic mode traveling through the ZnO layer [2]. We attribute this enhancement of the propagation lenght to the extended field distribution within the structure.

[1] S. Henn *et al.*, New J. Phys. **23**, 093031 (2021).
[2] S. Henn *et al.*, Appl. Phys. Lett. **125**, 211104 (2024).

HL 26.43 Wed 9:30 P1

Comparative *ab initio* characterization of $LiNbO_3$, Li_3NbO_4 and $LiNb_3O_8$ — •Frederik Schmidt and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Ferroelectric lithium niobate ($LiNbO_3$) is an important material for nonlinear optical technologies. It is part of the Li_2O–Nb_2O_5 system, whose two components can not only form $LiNbO_3$ but also other phases with different Li:Nb ratios, such as Li_3NbO_4 or $LiNb_3O_8$. Both are studied as possible materials for lithium-ion batteries on their own, but they may also occur as unwanted secondary phases during the growth of lithium niobate crystals when pure $LiNbO_3$ is preferred. As a consequence, it is important to detect and identify the different phases. In this work, we employ *ab initio* methods including density-functional theory, the *GW* approximation and the Bethe-Salpeter equation in order to characterize the three compounds with identical computational techniques and convergence parameters. In particular, we compare the density of states, electronic band structure and optical absorption spectrum of Li_3NbO_4 and $LiNb_3O_8$ to $LiNbO_3$. Despite qualitative similarities, our results reveal quantitative differences in the electronic and optical properties that should be clearly measurable in experiments. Compared to $LiNbO_3$, the electronic band gap of Li_3NbO_4 is 1.0 eV larger and that of $LiNb_3O_8$ is 0.4 eV smaller. The optical absorption edges also vary correspondingly.

HL 26.44 Wed 9:30 P1

Improving the optical readout of NV-centers in diamond by oxide surface coating — •Klemens Wurl, Michael Bar, Holger von Wenchstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute, Germany

Successful quantum computing has many advantages compared to regular computing, especially in simulations. It is proposed that nitrogen-vacancy (NV) centers in diamond could be used as qubits at room temperature, which would make everyday applications of quantum computing easier compared to solutions that rely on superconductivity.[1] The quantum states of the NV-centers can be controlled by optical excitation via laser and spin-state manipulation by microwave radiation.[2] The main objective of this research is to improve the optical readout of the NV-center by the use of solid immersion lenses (SIL). For this purpose, transition metal oxides are used, which are optically transparent and do not exhibit photoluminescence for the given wavelength. PLD is used for the surface coating, but the optical properties are limited by particle density. Therefore, peripheral target ablation was used to decrease the particle density as it allows for higher control of the plasma plume deflection. The influence of O_2 partial pressure and fluence will be investigated in order to record the corresponding growth window for decreased particle expulsion as well as increased optical transparency and refractive index.

[1] S.Pezzagna *et al.*, Appl. Phys. Rev. **8**(1), 011308, (2021).
[2] F. Jelezko *et al.*, Phys. Stat. Sol.(a) , **203**(13), 3207-3225, (2006).

HL 26.45 Wed 9:30 P1

Two-color sensitive II-VI wide-bandgap diodes with PbTe quantum dots for visible and infrared detection and emission — •Jakub Gluch[1], Sergij Chusnutdinow[1], Michal Szot[1,2], Piotr Wojnar[1], and Grzegorz Karczewski[1] — [1]Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland — [2]International Research Center MagTop, 02-668 Warszawa, Poland

We present the results of research on p-n diode working as two-color photodetector, made from combined narrow- and wide-bandgap semiconductors. With the use of molecular beam epitaxy (MBE) we managed to create diode structures (p-ZnTe/(Active Layers - AL)/n-CdTe) with lead telluride (PbTe, 0.32 eV in 300K) quantum dots embedded in cadmium telluride matrix (CdTe, 1.49 eV in 300K). To create quantum dots we first grown 20 alternating layers of PbTe and CdTe on top of p-type layer, which followed by thermal annealing which break down PbTe layers in to dots. We performed current-voltage measurements for the basic characteristics followed by an optical measurements to obtain diode spectral response curves with respect to different temperatures in the visible and infrared ranges (350 - 3500nm in 300K). In photoluminescence measurement we observe emission from PbTe quantum dots. We confirmed junction formation in the diode by electron beam induced current (EBIC) measurements. On cross sections of this structures, we observed formation of double p-n junction at the interface of p-type layer and AL, and AL and n-type layer. Measurements show promising possibilities for creating infrared LED and at the same time photodetector with wide spectrum of detectivity.

HL 26.46 Wed 9:30 P1

Microscopic reverse-bias electroluminescence spectra and spectral images of 850 nm oxide-confined VCSELs during burn-in — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Sebastian Haberkern[1], Helmut Meinert[1], Alexander Moll[1], Dominik Ölke[1], Ilya E. Titkov[2], Oleg Yu. Makarov[2], and Nikolay Ledentsov[2] — [1]Esslingen University of Applied Sciences, Flandernstrasse 101, 73732 Esslingen, Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Germany

850 nm vertical-cavity surface-emitting lasers (VCSELs) are studied during high-current burn-in operation utilizing both reverse-bias electroluminescence (ReBEL) spectra and spectral images. High-resolution spectral images are generated by means of a confocal scanning optical microscope using interference filters whereas microscopic spectra are obtained with a fiber-coupled sensitive USB spectrometer. Recently unfiltered ReBEL images have proven to be sensitive to operation-induced changes of VCSELs because defect states evolved during high-current stress trigger avalanche breakdown and give rise to ReBEL emission. In particular, local current crowding during high current burn-in leads to spatial distributions of ReBEL emission being characteristic to the aging status and contain spectral portions due to quantum well as well as AlGaAs barrier emissions. In contrast, electroluminescence spectra measured under near flatband conditions exhibit only quantum well emission at 848 nm.

HL 26.47 Wed 9:30 P1

Optical Properties of a Transition-metal Dichalcogenide - ZnO Nanowire Field-effect Transistor — •Yashvi Bulsara[1], Maximilian Tomoscheit[1], Omid Ghaebi[1], Edwin Eobaldt[1], Carsten Ronning[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, University of Jena — [2]Abbe Center of Photonics, University of Jena

Transition-metal dichalcogenide (TMD) monolayers combined with zinc-oxide (ZnO) nanowires (NW) represent a promising platform for electrically tunable nanophotonic devices. ZnO NWs are naturally nanoscale lasers, supporting waveguiding, field amplification and being the gain medium at the same time. A further major step towards the success and broad applicability of NW lasers is the possibility to actively tune their laser properties via external stimuli, such as the piezo-electric effect[2]. Recently, we have demonstrated that coupling of ZnO NWs to monolayer TMDs leads to an increase of the lasing intensity threshold[3]. Building on this approach. in this poster I will propose a device where the laser emission of a ZnO NW can be electrically tuned by coupling it to a TMD based field-effect transistor. Besides the main idea and device architecture, I will present preliminary results of device fabrication and characterization. [1] M. Zapf, Nano Lett., 2017, 17 (11), 6637-6643 [2] E. Eobaldt, Nanoscale, 2022,14, 6822-6829.

HL 26.48 Wed 9:30 P1

PT-Symmetry in Excitonic Spectra of TMDC Monolayers under Influence of Magnetic Fields — •Michiel Snoeken, Andreas Knorr, and Henry Mittenzwey — Nichtlineare Optik und Quantenelektronik, Institut für Physik und Astronomie (IFPA), Tech-

nische Universität Berlin, D-10623 Berlin, Germany

Excitons in TMDC monolayers under the influence of an in-plane magnetic field are theoretically studied. We demonstrate that in-plane magnetic fields induce a hybridization between spin-bright and spin-dark exciton transitions, resulting in a brightening of spin-dark excitons in optical experiments. We provide a thorough analytical characterization of the spectrum and demonstrate that, upon including dissipation, such a system can be interpreted as a gain-loss system as described in PT-symmetric quantum mechanics.

HL 26.49 Wed 9:30 P1

Calculation of thermodynamic potentials and heat capacities of ScN , YN and Au_2InYb — •Clemens Vogel and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik

ScN and YN can be incorporated in AlN to improve piezoelectric properties and electromechanical coupling. The Heusler phase Au_2InYb is of interest due to its potential for thermoelectric properties. In this work we computed the thermodynamic potentials, the entropy, the specific heat capacities C_p and C_V, and the thermal expansion coefficient. The calculations were performed using DFT/DFPT in Quantum ESPRESSO (PBE-XC) using the quasi-harmonic approximation for phonons. C_p and C_V were determined over the range of 3-600 K, as well as entropy and thermal expansion coefficient; C_p exceeds the Dulong-Petit limit. For Au_2InYb, the projected density of states was also calculated, which reveals a strong $4f$ density of states near the Fermi level and indicating valence fluctuation (in agreement with experimental findings); the calculated heat capacities agree very well with the experimental measurements.

HL 26.50 Wed 9:30 P1

Super-Resolution Terahertz Spectroscopy via Near-Field Electro-Optic Sampling — •Kevin Berwagner, Moritz Heindl, Fabian Brütting, and Georg Herink — Universität Bayreuth

Electro-optic sampling of THz radiation transmitted through a specimen provides a non-invasive way to analyze materials, however, the spatial resolution is typically constrained by the diffraction limit of the THz beam to a few hundred microns.

In this contribution, we will present our progress in developing a novel method for sampling pulsed terahertz fields with potentially submicron spatial resolution. Specifically, the approach is based on local imaging of THz nearfields via an electro-optic material in close contact with the specimen. In contrast to established near-field approaches, the method does not require the scanning of local probes such as SNOM or micro-antennas. We analyze phase-matching conditions and effective resolutions, and we demonstrate the super-resolution capabilities.

HL 26.51 Wed 9:30 P1

Highspeed ultrafast spectroscopy via active synchronization of dual-comb lasers — •Simeon Schmitt, Julia Lang, and Georg Herink — University of Bayreuth, Germany

Dual-comb lasers enable ultrafast spectroscopic measurements at high speeds by generating optical delays without the motion of mechanical elements. According to the asynchronous optical sampling (ASOPS) scheme, pulses from two mode-locked lasers with detuned repetition rates are combined to automatically scan relative delays throughout the pulse period. In contrast, here, we present a novel approach which features flexible active synchronization of both lasers: Employing precisely timed electrical signals and fast electro-optical modulators, we achieve full control over the overall scanning process. This concentrates the scanning range to the region of interest by limiting it to several picoseconds, resulting in record fast scanning rates. Furthermore, the scanning resolution can be arbitrarily adjusted up to tens of THz by varying the repetition rate difference. We adopt this process to realize ultrafast acquisition speeds for rapid THz time domain spectroscopy and present first measurements.

HL 26.52 Wed 9:30 P1

Ultrafast negative thermal expansion in NbO_2 — •Florian Baltrusch[1], Marc Herzog[1], Florin Boariu[2], Matthias Rössle[2], Jutta Schwarzkopf[3], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Niobium dioxide (NbO_2) exhibits negative thermal expansion (NTE), meaning it contracts upon heating rather than expanding like most materials. Below 200 K, bulk NbO_2 shows a monotonic contraction of the tetragonal c-axis, while the a/b-axes expand. This behaviour not only enables zero-expansion composites but also provides an unconventional elastic driving mechanism for magneto-elastic materials on picosecond timescales.

In epitaxial thin films, however, the lattice response is modified by substrate constraints via the Poisson effect. Temperature-dependent XRD measurements show that the film response depends strongly on the thermal-expansion mismatch between film and substrate during equilibrium heating.

Using ultrafast X-ray diffraction (UXRD), we directly observe ultrafast NTE in NbO_2 thin films. On picosecond timescales, the substrate remains effectively "frozen", allowing us to isolate the intrinsic response of the NbO_2 layer. This enables us to determine the timescale of contraction, which provides crucial insights about its driving mechanism.

HL 26.53 Wed 9:30 P1

Development of single-shot spectral referencing to increase signal-to-noise ratio in broadband 2D electronic spectroscopy — •Lotte Polling, Anton Trenczek, Pavel Trofimov, Trideep Kawde, and Hélène Seiler — FU Berlin

Two-dimensional optical spectroscopy is a powerful technique for resolving couplings between electronic states. Its implementation relies on the availability of a broadband light source in the visible range, typically generated using non-collinear optical parametric amplifiers or gas-filled hollow-core fibers. These sources exhibit shot-to-shot spectral fluctuations which can be as high as 10-15% depending on the laser source. Here, we introduce a setup for single-shot spectral referencing with the end goal of significantly increasing the signal-to-noise ratio in broadband 2D electronic spectroscopy measurements.

HL 26.54 Wed 9:30 P1

Ultrafast Lattice Dynamics in Gold Beyond the Kinematic Approximation — •Helena Hollstein[1,2], Sebastian Hammer[2], and Heinrich Schwoerer[1] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany — [2]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

In the interpretation of electron diffraction experiments, the kinematic scattering approximation and simple phonon models are often used to reduce computational cost when modeling structural dynamics [1]. However, even for well-studied benchmark systems such as polycrystalline gold thin films, it often remains unquestioned how reliably these assumptions hold under strong nonequilibrium excitation [2].

In this work, we investigate a 20 nm gold thin film under optical excitation using ultrafast electron diffraction (UED) and static temperature dependent electron diffraction to extract transient atomic displacements and determine phonon excitation by analyzing the Debye-Waller effect. We compare our experimental findings of lattice heating dynamics with simulated diffraction patterns that rely on kinematic scattering and harmonic phonon models. We hereby assess to what extent the commonly used theoretical frameworks cease to describe the structural response accurately. Our findings demonstrate that neglecting possible anharmonic potentials, phonon-phonon coupling and multiple scattering-effects can lead to systematic misinterpretations of ultrafast lattice dynamics and thermophysical material properties.

[1] Schäfer et al. *Chem. Phys. Lett.* **515** (2011)
[2] Durham et al. *Struct. Dyn.* **9** 064302 (2022)

HL 26.55 Wed 9:30 P1

Ultrafast dynamics of exciton–exciton interaction in monolayer MoS_2 investigated by high-order pump–probe microspectroscopy — •Ruidan Zhu, Patrick Grenzer, Simon Büttner, Matthias Hensen, Tobias Hertel, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Exciton–exciton interaction (EEI), as a many-body effect, sets a fundamental limit to optimizing the photoluminescence efficiency of light-emitting devices based on 2D materials under high exciton densities [1]. A detailed understanding of the underlying EEI mechanisms provides crucial insight for the optimization of the device performance. However, EEI dynamics are challenging to probe directly as their signatures are mixed with the dominant single-exciton background in conventional ultrafast measurements. Here, we apply our recently developed high-order pump–probe spectroscopy [2] in a cryo-microscope to study exciton interaction in freestanding and supported MoS_2 monolayers. We aim to separate different EEI-related processes (fifth and higher orders of the system's nonlinear response) from the single-exciton dy-

namics (third order) and further investigate how the dielectric environment influences EEI dynamics. We present our current progress toward isolating EEI dynamics.

[1] Y. Yu et al., Phys. Rev. B 2016, 93, 201111.
[2] P. Malý et al., Nature 2023, 616, 280.

HL 26.56 Wed 9:30 P1

Impulsive Stimulated Raman Scattering: Highspeed Detection Strategies — •Laura Hüllmandel, Julia A. Lang, and Georg Herink — Universität Bayreuth

Pulse interaction of femtosecond pulses inside Ti:Sapphire lasers is mediated by Raman-active modes with terahertz beats causing bound states of solitons at fixed time delays [1]. In this contribution, we employ extra-cavity impulsive stimulated Raman scattering (ISRS) to quantitatively determine the phase-shifts involved to further our understanding of the intra-cavity formation of so-called "soliton molecules". We compare spectral-shift and interferometric methods for phase-sensitive detection and achieve efficient noise reduction of multiplicative $1/f$ noise sources – where lock-in amplification is ineffective – through rapid scan-averaging and balanced detection.

[1] A. Völkel et al., "Intracavity Raman Scattering Couples Soliton Molecules with Terahertz Phonons.", Nature Communications 13.1 (2022).

HL 27: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

HL 27.1 Wed 10:30 TRE/MATH

Polarons in epitaxial single-layer $MnBr_2$ — •Affan Safeer, Oktay Güleryüz, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We investigate polaron formation in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates: graphene on Ir(110), graphene on Ir(111), and Au(111). The polaron number densities and species depend strongly on the underlying substrate, underscoring the crucial role of the substrate. Our findings show that modeling of polarons in such single-layer insulators in contact with conducting substrates must explicitly include the substrate. For $MnBr_2$ grown on graphene/Ir(110), we identify four distinct polaron species, three of which closely resemble those reported for $CoCl_2$ on graphite. These polarons can be created, converted, and laterally manipulated by the STM tip when a tunneling current flows at suitable bias voltages. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided by the periodic potential imposed by the supermoiré pattern arising from the interaction of $MnBr_2$ with graphene and Ir(110).

HL 27.2 Wed 10:45 TRE/MATH

Chirality in the Kagome Metal CsV_3Sb_5 — •Tom P. Lammerskötter[1], H.J. Elmers[2], G. Schönhense[2], O. Tkach[2], Y. Lytvynenko[2], H. Agarwal[2], S. Chernov[3], M. Hoesch[3], D. Kutnyakhov[3], M. Scholz[3], K. Rossnagel[4], A. Gloskovskii[3], C. Schlueter[3], A. Winkelmann[5], A. Haghighirad[6], M. Schmitt[7], T. Lee[7], R. Claessen[8], M. Le Tacon[6], J Demsar[2], and O. Fedchenko[1] — [1]Goethe-Universität Frankfurt (Germany) — [2]JGU Mainz (Germany) — [3]DESY Hamburg (Germany) — [4]Universität zu Kiel (Germany) — [5]AGH University of Krakow (Poland) — [6]KIT Karlsruhe (Germany) — [7]DIAMOND (UK) — [8]Universität Würzburg (Germany)

Kagome metals AV_3Sb_5 (A = Cs, K, Rb) exhibit flat bands, Dirac points, and van Hove singularities that drive unconventional charge-density-wave (CDW) order and topological states. We study chirality in CsV_3Sb_5 using angle-resolved photoemission spectroscopy (ARPES) and x-ray photoelectron diffraction (XPD) with circularly polarized photons. XPD reveals a local crystal chirality in the CDW phase. ARPES shows pronounced magnetic circular dichroism (MCD), demonstrating a chiral electronic structure and indicating orbital moments possibly linked to loop-current order. To probe orbital-moment coupling, we study Nb-doped CsV_3Sb_5, where band broadening and enhanced Dirac-like gaps occur. In the CDW phase, the strongly increased MCD indicates time-reversal-symmetry breaking and couples to the three van Hove singularities at the M points.

HL 27.3 Wed 11:00 TRE/MATH

Ab initio and group theory ananlysis of monolayer BiTeI — •Josep Mas-Garcia, Jorge Cervantes-Villanueva, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV - University of Valencia - Spain

Monolayer BiTeI is a prototypical polar semiconductor whose remarkable Rashba spin splitting, rooted in strong spin-orbit coupling and non-centrosymmetric structure, offers a fertile landscape for advancing two-dimensional spintronics. This work presents and ab initio and group-theoretical analysis of BiTeI. Employing fully relativistic density functional theory and GW calculations, we obtain electronic structures that serve as benchmarks for the group-theory based Hamiltonian model. Leveraging the systematic method of invariants, we construct symmetry-constrained k-p Hamiltonians near the Γ point. Our implementation of the method of invariants enables precise fitting of the Hamiltoninan eigenvalues to ab initio band dispersions for the obtention of the parameters, and yields a highly compact analytic model that reproduces Rashba splitting and symmetry-dependent features. This framework facilitates straightforward evaluation of key physical quantities, such as effective masses or spin textures, and perturbative responses including electric and magnetic fields and strain effects within a unified and transparent formalism. Moreover our methodology establishes a versatile template for the symmetry-guided modeling of nonmagnetic semiconductors with strong spin-orbit coupling.

HL 27.4 Wed 11:15 TRE/MATH

Production of Interstitials in 2D Transition-Metal Dichalcogenides (TMDs) by Ion Irradiation: ab-initio Simulations — •Silvan Kretschmer[1], Joel Davidsson[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark — [2]Department of Physics, Linköping University, Sweden

Defects critically shape the properties of two-dimensional (2D) materials and can be purposefully introduced to tune magnetic, electronic, and optical behavior. Low-energy ion irradiation has recently emerged as an effective route for generating specific defect types via direct implantation [1,2].

First-principles simulations are essential for understanding irradiation-induced defect formation [3], but DFT-based molecular dynamics (MD) is computationally costly and limits broad exploration of materials and irradiation conditions. Machine-learning (ML) interatomic potentials provide a high-accuracy, low-cost alternative, enabling efficient screening of large datasets such as the Impurities in 2D Materials Database [4].

Here, we benchmark a ML potential against ab-initio MD, emphasizing accurate treatment of the short interatomic distances occurring during ion impacts. We apply the fine-tuned ML to study interstitial defect formation in TMDs under low-energy ion irradiation, providing defect formation probabilities and identifying suitable ion-beam parameters for targeted defect engineering in 2D materials.

[1] 10.1038/s41699-022-00318-4 [2] 10.1021/acsnano.4c03475
[3] 10.1103/PhysRevMaterials.8.114003 [4] 10.11583/DTU.19692238

HL 27.5 Wed 11:30 TRE/MATH

Long-living metastable electronic states in substituted $1T$-TaS_2 — •Gaël Reecht[1], Jesumony Jayabalan[1], Ričards Knipšis[2], Florian Diekmann[3], Friedemann Queisser[2], Ping Zhou[1], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]University Duisburg-Essen, Germany — [2]HZ Dresden-Rossendorf, Germany — [3]CAU of Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]DESY, Hamburg, Germany

$1T$-TaS_2 is a prototypical correlated material whose low-temperature phase exhibits a commensurate charge density wave forming Star-of-David (SOD) clusters. Each SOD hosts a single electron close to E_F and, due to strong on-site Coulomb repulsion, the system enters a Mott insulating state. Adding or removing an electron creates doublon or holon excitations, which typically relax within few femtoseconds [1]. Here, we manipulate the lifetime of the quasiparticle exci-

tations by substituting some Ta with an electron richer element. Using LT-scanning tunnelling microscopy and spectroscopy (STM/STS) and time-resolved photoemission spectroscopy, we observe metastable doublons with lifetimes ranging from fs to hours. STM/STS further shows that these excitations are locally confined. The experimental observations are corroborated by a theoretical description based on a Fermi-Hubbard model. The disorder induced by the random substitution leads to a spatial localization of holon and doublon wavefunctions at the origin of the long lifetimes observed experimentally.

[1] M. Ligges et *al.*, Phys. Rev. Lett., **120**, 166401 (2018)

HL 27.6 Wed 11:45 TRE/MATH

Fingerprints of Excitonic Collective Modes in the Two-Dimensional Electron Gas — •Jakob Wolff[1,2,3], Silvana Botti[2,3], Lucia Reining[4,3], and Matteo Gatti[4,3,5] — [1]Institut für Festkörpertheorie- und Optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems, University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]LSI, CNRS, CEA/DRF/IRAMIS, École polytechnique, Institut Polytechnique de Paris, France — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

We investigate the collective charge excitations of the two-dimensional homogeneous electron gas in the low density regime within the framework of time-dependent density functional theory. We show that beyond the well-known plasmons new collective excitonic modes emerge, which leave characteristic fingerprints in experimentally accessible quantities, such as asymmetric peak structures in the loss function and enhanced Friedel oscillations. Further, at sufficiently low densities the collective modes become imaginary, indicating an instability towards the formation of a charge-density-wave phase with excitonic origin.

HL 27.7 Wed 12:00 TRE/MATH

Moir'e modulated quantum spin liquid candidate 1T-TaSe2 — Ziying Wang, Adolfo O. Fumega, Ana Vera Montoto, Mohammad Amini, Büsra Gamze Arslan, Ales Cahlik, Yuxiao Ding, Jose L. Lado, •Robert Drost, and Peter Liljeroth — Aalto University, Department of Applied Physics

Quantum spin liquids continue to fascinate with their highly entangled quantum states and promises of fractional many-body excitations. Yet there are few tools to probe these materials, and none sensitive enough for applications in 2D materials. This seriously hampers the study of monolayer QSL candidates such as α-RuCl3 and 1T-TaSe2. Scanning tunneling microscopy and spectroscopy may overcome this challenge, as they can access the fundamental excitations of 2D samples through inelastic tunneling spectroscopy. These low-energy excitations can be compared against theoretical models and provide fingerprints of QSL states. We employ this approach against the quantum spin liquid candidate 1T-TaSe2. We observe the emergence of a root 3 reconstruction driven by the substrate, equivalent spectroscopy across all spin sites, and the coexistence of zero and finite energy excitations. These observations are consistent with a QSL ground state. Our results demonstrate that IETS provides a powerful route to obtain atomic-scale insight into the magnetic excitations of two-dimensional materials. Spectral fingerprints may help to identify exotic phases of matter that are otherwise difficult to detect.

HL 27.8 Wed 12:15 TRE/MATH

Long-Range Interactions in Twisted Bilayer Materials with Machine Learning for the Electronic Density — •Zekun Lou[1], Alan Lewis[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of York, York, U.K.

Moiré superlattices in twisted bilayer (TB) 2D materials exhibit extraordinary quantum phenomena, but first-principles understanding remains limited by computational costs. While most machine learning (ML) methods for density functional theory (DFT) acceleration are based on the locality assumption, we demonstrate that accurate moiré electronic structure prediction requires long-range encoding due to charge rearrangement, orbital hybridisation, and moiré potential modulation. Using long-range representations [1] for electronic-density prediction [2,3], we achieve low-energy band-structure predictions with <15 meV errors across twisted bilayer graphene (TBG), hBN, and transition-metal dichalcogenides (TMDCs), while ∼100 times faster than DFT. Descriptor requirements are material-dependent: homoatomic systems (e.g., TBG) are well-described by local descriptors, while hBN and TMDCs require long-range encoding. We summarise the physical implications of these findings that marry machine learning and the fundamental physics that governs the electronic density of twisted bilayer materials.

[1] A. Grisafi, M. Ceriotti, JCP 151, 204105 (2019)
[2] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, JCTC 17, 7203 (2021)
[3] A. Grisafi, A. Lewis, M. Rossi, M. Ceriotti, JCTC 19, 4451 (2023)

HL 28: Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0401

HL 28.1 Wed 15:00 HSZ/0401

Majorana or Not? An Insight from Atomic-Scale Shot-Noise — •Abhishek Maiti[1], Genda Gu[2], and Freek Massee[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France — [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA

The search for non-abelian states of matter has become a central theme of modern quantum material research. Notably, Majorana zero modes are of special interest, as they can serve as the foundation for topological qubits. A robust zero-bias conductance peak, observed in scanning tunneling spectra, is often regarded as the primary signature of a Majorana zero mode. Yet similar features can also arise from trivial bound states, raising a long-standing challenge of how to distinguish a genuine Majorana from imposters. In my talk, I will address this problem with a new approach, atomic-scale shot-noise spectroscopy, that goes beyond conductance measurements. Through a detailed investigation on multiple defect- and vortex-bound zero-bias states in the widely studied (putative) topological superconductor Fe(Se,Te), I will show that while differential conductance measurements might sometimes fail to detect an imposter Majorana state locally, noise measurements consistently provide a conclusive diagnostic, offering a powerful complementary probe. Looking ahead, this technique can be applied to other reported platforms to verify whether their Majorana-like signature in tunneling conductance can pass the shot-noise test.

HL 28.2 Wed 15:15 HSZ/0401

Intrinsic topological superconductivity revealed by surface-extended Andreev bound states in $PtBi_2$ — •Xiaochun Huang[1], Lingxiao Zhao[2], Sebastian Schimmel[3,4], Julia Besproswanny[3,4], Patrick Härtl[1], Christian Hess[3,4], Bernd Büchner[4,5], and Matthias Bode[1] — [1]Experimentelle Physik 2, Physikalisches Institut, Universität Würzburg, Germany — [2]Quantum Science Center of Guangdong, Shenzhen, China — [3]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Germany — [4]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [5]Technische Universität Dresden, Germany

Intrinsic topological superconductivity remains a central question in condensed-matter physics. The three-dimensional Weyl semimetal $PtBi_2$ was recently shown by angle-resolved photoemission spectroscopy to host a superconducting gap that opens exclusively on its Fermi-arc surface states with a nodal structure, establishing it as a prime candidate for intrinsic topological superconductivity [1]. Using scanning tunneling microscopy and spectroscopy, we directly visualize surface-extended Andreev bound states (ABSs) across atomically pristine terraces within a sizable superconducting gap ($\Delta > 10\,\mathrm{meV}$) in $PtBi_2$. Quantitative analysis of the tunneling spectra within an anisotropic chiral pairing framework identifies these ABSs as signatures of an emergent Majorana-cone dispersion. Our findings provide a definitive real-space spectroscopic fingerprint of intrinsic topological superconductivity in $PtBi_2$.

[1] A. Kuibarov *et al.*, Nature **626**, 294 (2024)

HL 28.3 Wed 15:30 HSZ/0401

Probing chiral symmetry with a topological domain wall sensor — •Artem Odobesko[1], Glenn Wagner[2], Titus Neupert[2], Ronny Thomale[1], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, University of Zurich, Zürich, Switzerland

Chiral symmetry is a fundamental property with profound implications for the properties of elementary particles, that implies a spectral symmetry (i.e. E -> -E) in their dispersion relation. In condensed matter physics, chiral symmetry is frequently associated with superconductors or materials hosting Dirac fermions such as graphene or topological insulators. There, chiral symmetry is an emergent low-energy property, accompanied by an emergent spectral symmetry. While the chiral symmetry can be broken by crystal distortion or external perturbations, the spectral symmetry frequently survives. As the presence of spectral symmetry does not necessarily imply chiral symmetry, the question arises how these two properties can be experimentally differentiated. Here, we demonstrate how a system with preserved spectral symmetry can reveal underlying broken chiral symmetry using topological defects. Our study shows that these defects induce a spectral imbalance in the Landau level spectrum, providing direct evidence of symmetry alteration at topological domain walls. Using high-resolution STM/STS we demonstrate the intricate interplay between chiral and translational symmetry which is broken at step edges in topological crystalline insulator $Pb_{1-x}Sn_xSe$.

[1] G. Wagner et al., Newton **1**, 100009 (2025)

HL 28.4 Wed 15:45 HSZ/0401

Quantifying quasiparticle chirality in a chiral topological semimetal — •Jiaju Wang[1], Amit Kumar[1], Markel Pardo-Almanza[1], Jaime Sanchez-Barriga[2], Jorge Cardenas-Gamboa[3], Maia Vergniory[3], Vladimir Strokov[4], Moritz Hoesch[5], Chandra Shekhar[6], Claudia Felser[6], Stuart Parkin[1], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, electron chirality has been proposed as an order parameter to quantify chirality. In chiral topological semimetals with the B20 structure, electron chirality is linked to parallel spin-momentum locking (SML) and spin deviations from SML, which affects numerous physical properties. However, experimental quantification of spin deviation still remains a big challenge. To achieve this, we have used spin and angle-resolved photoemission spectroscopy to directly probe the spin texture of Weyl cones in RhSi, a chiral topological semimetal with strong spin-orbit coupling (SOC). The spin-resolved spectra at different azimuthal angles are intricately fitted to extract numerical values of spin deviation for Weyl cones, allowing us to calculate the normalized electron chirality density (NECD). It was found that deviations can decrease the NECD from 1 down to 0.8. This observation may help interpret physical phenomena in chiral topological semimetals.

HL 28.5 Wed 16:00 HSZ/0401

Topology and Real-Space Obstruction: The Phase Diagram of the Triangular p-Orbital Lattice — •Jonas Erhardt[1,2], Sven Schemmelmann[3], Fabian Schöttke[3], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,4], Markus Donath[3], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ctd.qmat — [3]Physikalisches Institut, Universität Münster — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Triangular p-orbital monolayers (MLs) host a rich topological phase diagram governed by the competition between spin-orbit coupling (SOC) and substrate-induced inversion-symmetry breaking (ISB). The SOC-dominated quantum spin Hall insulator (QSHI) phase arises from a band inversion in the $p_\pm$ manifold and was first realized in indenene, a triangular ML of In atoms on SiC [1]. Real-space interference shifts the associated Wannier centers away from the atoms to interstitial sites A/B, which for the QSHI phase produces an alternating ABAB energy sequence in the charge localization, as demonstrated by scanning tunneling microscopy (STM) [1]. Using the same STM approach, we identify the complementary ISB-dominated regime in a Tl ML on Si(111), where strong adsorption-induced ISB exceeds Tl's SOC. The charge likewise shifts off the atoms but evidences a non-alternating AABB sequence, characterizing Tl/Si(111) as a trivial obstructed atomic insulator. These results complete the experimental validation of the topological phase diagram for triangular p-orbital MLs.

[1] Nat. Commun. **12**, 5396 (2021).

HL 28.6 Wed 16:15 HSZ/0401

Majorana-metal transition in a disordered superconductor: percolation in a landscape of topological domain walls — Vladimir A Zakharov[1], Ion Cosma Fulga[2,3], •Gal Lemut[4], Jakub Tworzydło[5], and Carlo W. J. Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, PO Box 9506, 2300 RA Leiden, The Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany — [4]Dahlem Center for Complex Quantum Systems and Physics Department, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [5]Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warszawa, Poland

Most superconductors are thermal insulators. A disordered chiral p-wave superconductor, however, can make a transition to a thermal metal phase. Because heat is then transported by Majorana fermions, this phase is referred to as a Majorana metal. Here we present numerical evidence that the mechanism for the phase transition with increasing electrostatic disorder is the percolation of boundaries separating domains of different Chern number. We construct the network of domain walls using the spectral localizer as a "topological landscape function", and obtain the thermal metal-insulator phase diagram from the percolation transition.

HL 28.7 Wed 16:30 HSZ/0401

fabrication and characterization of the Moiré surface state on a topological insulator — •yi zhang — Shanghai Jiao Tong University, Shanghai, China

A Moire* superlattice on the topological insulator surface is predicted to exhibit many novel properties but has not been experimentally realized. Here, we developed a two-step growth method to successfully fabricate a topological insulator Sb2Te3 thin film with a Moire* superlattice, which is generated by a twist of the topmost layer via molecular beam epitaxy. The established Moire* topological surface state is characterized by scanning tunneling microscopy and spectroscopy. By application of a magnetic field, new features in Landau levels arise on the Moire* region compared to the pristine surface of Sb2Te3, which makes the system a promising platform for pursuing next-generation electronics. Notably, the growth method, which circumvents contamination and the induced interface defects in the manual fabrication method, can be widely applied to other van der Waals materials for fabricating Moire* superlattices.

HL 28.8 Wed 16:45 HSZ/0401

Backscattering in topological edge states despite time-reversal symmetry — Jonas Erhardt[1,2], •Mattia Iannetti[3,4], Fernando Dominguez[2,5], Ewelina M. Hankiewicz[2,5], Björn Trauzettel[2,5], Gianni Profeta[3,4], Domenico Di Sante[6], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [4]CNR-SPIN C/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [6]Department of Physics and Astronomy, University of Bologna

Quantum Spin Hall Insulators (QSHI) are promising materials for many applications based on Dirac fermions and topologically-protected edge states. Indium adatoms on a silicon carbide surface, the so-called Indenene, was the first material in which a topological classification solely based on an inspection of the bulk wave functions has been demonstrated. In this work, we present a combined experimental and theoretical study of finite-sized Indenene systems, using STM/STS measurements and a quantitative tight-binding model revealing the rich physics of edge states. We find that a strongly non-linear edge dispersion leads to inter-Kramers pair backscattering, thereby extending the conventional understanding of backscattering protection in topological edge states.

HL 28.9 Wed 17:00 HSZ/0401

Quantized Subband Tunneling from Topological Insulator Nanowire Scanning Probe Tips — •Abhisek Kole[1,2], Felix

Münning[3,4], Xiaosheng Yang[1,5], Jia G. Lu[6], Oliver Breunig[4], F. Stefan Tautz[1,2], Yoichi Ando[4], and Felix Lüpke[1,4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Experimental Physics IV A, RWTH Aachen University, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Institute of Physics I, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [4]Institute of Physics II, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [5]School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China — [6]Department of Physics/Electrophysics, University of Southern California, Los Angeles, CA 90089, USA

In topological insulator nanowires, the interplay between size quantization and the surface states wrapping the nanowire circumference gives rise to a magnetic-flux-tunable band structure. We demonstrate the controlled fabrication of (Bi_(1-x) Sb_x)_2 Te_3 (BST) topological insulator nanowires into scanning tunneling microscopy tips. Tunneling spectroscopy reveals a series of distinct peak-like features that exhibit a characteristic 1D DOS, indicating tunneling into the quantized 1D subbands of the BST nanowire tips. Furthermore, a magnetic-field-induced gap-closing and reopening transition is observed, consistent with the Dirac-like gap-closing transition expected for such wires. Moreover, we find indications of spin-selective helical tunneling between the nanowire tip and the Rashba surface states of Au(111).

HL 28.10 Wed 17:15 HSZ/0401

Simultaneous Characterization of Dispersion and Orbital Character of the Topological Surface State on the Topological Insulator Bi_2Te_3 — •Christoph Stephen Setescak, Adrian Weindl, and Franz Josef Giessibl — Universität Regensburg, D-93053 Regensburg

Scanning probe microscopy (STM and AFM) allows one to locally probe properties of topological insulators (TIs). On the compound Bi_2Te_3, atomic-scale electronic standing waves can be observed at crystalline step edges, which are associated with the hexagonal warping of the Dirac cone. These real-space oscillations provide a direct means to study the dispersion relation of the topological boundary mode. The interpretation relies on comparing the experimental data to calculations including not only the properties of the TI but also of the tip. In this framework, the tunneling current and differential conductance is modelled using Chen's derivative rule. Bending of the CO molecule at the tip apex due to lateral tip-sample forces is also included in the model. The relevant Bloch functions of the sample are obtained from Wannier-interpolated tight-binding Hamiltonians using maximally localized Wannier functions derived from first-principles DFT + *GW* computations. In combination with the high spatial resolution obtained with CO-terminated tips, not only the dispersion, but also the orbital character of the band structure can be probed.

HL 28.11 Wed 17:30 HSZ/0401

Defect-induced displacement of topological surface state in magnetic topological insulator $MnBi_2Te_4$ — •Felix Lüpke[1,2], Marek Kolmer[3,4], Hengxin Tan[5], Adam Kaminski[3,4], and Binghai Yan[5,6] — [1]Peter Grünberg Institute (PGI-3) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Ames National Laboratory, Ames, Iowa 50011, USA — [4]Iowa State University, Ames, Iowa 50011, USA — [5]Weizmann Institute of Science, Rehovot 7610001, Israel — [6]The Pennsylvania State University, University Park, Pennsylvania 16802, USA

The gapped topological surface states of $MnBi_2Te_4$ (MBT) are an attractive platform for the realization of quantum anomalous Hall and Axion insulator states. However, experimentally observed surface state gaps fail to meet theoretical predictions, with the exact mechanism behind the gap suppression still being debated. We report on the effect of intrinsic anti-site defects on the MBT surface states, which we study using scanning tunneling microscopy (STM), angle-resolved photoemission (ARPES), and density functional theory (DFT). Our results show that high defect concentrations lead to a displacement of the surface states into the interior of the MBT crystal, consistent with theoretical predicitons [PRL 130, 126702 (2023)].

HL 29: Quantum Transport and Quantum Hall effects (joint session HL/TT)

Time: Wednesday 15:00–16:15 Location: POT/0006

HL 29.1 Wed 15:00 POT/0006

High Harmonic Hall Currents Driven by Curved Conducting Nanoarchitecture — •Ching-Hao Chang[1,2], Botsz Huang[1,2], Wei-Xiang Yin[1,2], and Xiao Zhang[3] — [1]Department of Physics, National Cheng Kung University Tainan, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University Tainan 70101, Taiwan — [3]Institute for Theoretical Solid State Physics Leibniz Institute for Solid State and Materials Research Dresden Helmholtzstr. 20, D-01069 Dresden, Germany

We theoretically establish a realizable non-perturbative mechanism for generating high harmon- ics (up to 6th order) in Hall currents within curved two-dimensional nanoarchitectures. Unlike previously explored perturbative mechanisms based on inversion symmetry breaking or Berry curvature, the high-harmonic generation demonstrated here is driven by magnetic-field dipoles induced purely by nanoscale curvature under an applied uniform magnetic field. We develop a theory showing that these harmonics originate from unique snake orbits induced by the interplay between an alternating electric field and curvature-induced magnetic-field dipole. Moreover, we establish quantitative control over harmonic suppression and enhancement by tuning the amplitude and orientation of the magnetic field, uncovering distinct symmetry-based even/odd harmonic selection rules. These findings provide a tunable platform for engineering nonlinear currents in curved electronics, with potential applications in developing high-frequency Hall sensors and THz devices.

HL 29.2 Wed 15:15 POT/0006

Gate-tunable isospin switching in graphene Mach-Zehnder electronic interferometers — •Antonio Lacerda-Santos, Lilian Seyve, Yassine Setti, Bikash Barik, Leo Pugliese, Preden Roulleau, and Cosimo Gorini — SPEC, CEA, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Graphene has become an exciting platform for electron (quantum) optics experiments [1]. Compact electronic interferometers can be realised via p-n interfaces, which in quantizing magnetic fields host counter-propagating chiral edge states. In a paradigmatic architecture with a single junction, such quantum Hall states form a Mach-Zehnder interferometer [2, 3]. The precise position of such edge states is set by the electrostatics of a given device [4], which can be determined to great accuracy with the self-consistent Schrödinger-Poisson solver Pescado [5].

We perform electrostatic and quantum transport simulations accompanying conductance measurements in a graphene Mach-Zehnder interferometer, and show that remote gates can be used to control the position of the p-n junction on sub-nanometer scales. Such a fine control does not meaningfully affect the edge state positions and lengths, but induces valley-isospin oscillations. The interferometer thus behaves as a tunable valley-isospin transistor.

[1] H. Chakraborti et al., J.Phys.:Condens.Matter 36 (2024) 393001 [2] D.S.Wei et al, Science Advances 3, e1700600 (2017) [3] M. Jo et al, PRL 126, 146803 (2021) [4] I.M. Flor et al, PRB 105, L241409 (2022) [5] A. Lacerda-Santos, arXiv:2507.03131v1

HL 29.3 Wed 15:30 POT/0006

Phase-coherent autonomous nonequilibrium demon — •José Balduque[1,2] and Rafael Sánchez[1,2,3] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain. — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain — [3]Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain.

Mesoscopic conductors enable the efficient management and useful conversion of not only thermal resources but also nonequilibrium electron distributions. The latter scenario makes it possible to define demonic modes of operation, in which the entropy of a subsystem is autonomously reduced without extracting net particles or energy from the subsystem that provides the nonequilibrium resource [1]. We propose an implementation of such a nonequilibrium demon, or N-demon, in a multiterminal system that exploits carrier coherence. This

is achieved by directly coupling the demonic subsystem to an isothermal two-terminal conductor via a scanning tip, enabling the local injection of electrons in a nonthermal distribution that participates in the phase-coherent interference processes governing the system's transport response [2]. In this way, we uncover an extrinsic, nonlocal, and phase-tunable transport response induced by the demon [3].

[1] R. Sánchez, et al., Phys. Rev. Lett. 123, 216801 (2019).
[2] R. Sánchez, et al., Phys. Rev. B, 105, 239903 (2022).
[3] J. Balduque and R. Sánchez, in preparation.

HL 29.4 Wed 15:45 POT/0006

Exploring the Influence of Electron Density on the Giant Negative Magnetoresistance — •Lina Bockhorn[1], Christian Reichl[2], Werner Wegscheider[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases exhibit a robust negative magnetoresistance at zero magnetic fields, characterized by a temperature-independent peak around $B = 0\,\mathrm{T}$ and a temperature-dependent giant negative magnetoresistance (GNMR) at higher fields [1-4]. By varying the electron density in situ, we gain valuable insights into the nature of GNMR. Our study shows a significant dependence of GNMR on electron density, suggesting that scattering potential variations [5] may not be fully addressed in current theoretical models. By examining these dependencies for different temperatures, we enhance the understanding of unresolved aspects of GNMR theory, potentially bridging the gap between experimental observations and theoretical predictions.

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[3] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[4] L. Bockhorn et al., Phys. Rev. B 109, 205416 (2024).
[5] Y. Huang et al., Phys. Rev. Materials 6, L061001 (2022).

HL 29.5 Wed 16:00 POT/0006

A topological field-effect memristor — •Fabian Hartmann[1], Manuel Meyer[1], Selena Barragan[1], Sergey Krishtopenko[1,2], Jean-Baptiste Rodriguez[3], Eric Tournie[3], Benoit Jouault[2], Gerald Bastard[1], Frederic Teppe[2], Lukas Worschech[1], Victor Lopez-Richard[4], and Sven Höfling[1] — [1]Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg — [2]L2C, CNRS-Université de Montpellier, France — [3]IES, Université de Montpellier, France — [4]Departamento de Fisica, Universidade Federal de Sao Carlos, Brazil

Quantum and neuromorphic computing rely on unconventional materials and device functionalities, yet achieving resilience to imperfections and reliable operation remains a major challenge. This has motivated growing interest in topological materials that provide robust and low-power operation while preserving coherence. However, integrating topological transport with memory functionality into a reconfigurable device has remained elusive. Here, we realize a topological field-effect memristor in which topological protection preserves edge state coherence, enabling the coexistence of coherent transport and non-volatile memory functionality. Utilizing inverted InAs/GaInSb/InAs trilayer quantum wells, we realize a quantum spin Hall insulator that exploits its intrinsic floating-gate behavior. This feature allows one to reconfigure the conventional field-effect transistor operation into memristive functionality with broad electric-field tunability. One resistance state is entirely governed by dissipationless, coherent transport.

HL 30: 2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)

Time: Wednesday 15:00–17:15 Location: POT/0081

Invited Talk HL 30.1 Wed 15:00 POT/0081

Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures — •Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich — Munich Center for Quantum and Technology (MCQST)

The coexistence of induced spin-orbit coupling (SOC) and magnetic exchange fields is predicted to drive graphene into topological phases, such as the quantum anomalous Hall state. Here, I will discuss the prospect of using monolayer graphene proximitized by WSe_2 (SOC) and $Cr_2Ge_2Te_6$ (magnetic exchange) for such dual proximity control. To determine the type and strength of the induced SOC, I will compare Landau fan analysis, where level anticrossings can serve as direct signatures of spin-orbit splittings, to optoelectronic measurements on graphene/WSe_2 heterostructures, where the photogalvanic effect can provide an indirect fingerprint of SOC. Low-temperature magnetotransport measurements of the heterostructures with combined magnetic and SOC proximity reveal a large and gate-tunable anomalous Hall effect persisting at zero magnetic field, signaling an intrinsic Berry curvature arising from the interplay of SOC and magnetism. These results highlight the coexistence of spin-orbit and magnetic proximity effects in graphene-based van der Waals heterostructures and establish a route toward topological graphene phases.

HL 30.2 Wed 15:30 POT/0081

Twist angle and pressure tuning of proximity-induced spin-orbit coupling in graphene/WSe_2 heterostructures — Tobias Rockinger[1], Bálint Szentpéteri[2], Szabolcs Csonka[2], Marina Marocko[1], Julia Amann[1], Ziyang Gan[3], Antony George[3], Andrey Turchanin[3], Kenji Watanabe[4], Takashi Taniguchi[4], Dieter Weiss[1], Péter Makk[2], and •Jonathan Eroms[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [3]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [4]National Institute for Materials Science, Tsukuba, Japan

Proximity-induced spin-orbit interaction in heterostructures of graphene and transition metal dichalcogenides has been studied intensely in the past few years. However, present experiments still suffer from poor reproducibility, as one key parameter, the twist angle between the crystal axes of both materials, has not been systematically controlled during fabrication. Band structure calculations, on the other hand, have predicted a decisive influence of this parameter. In our experiments, we control the twist angle during fabrication by aligning fractured or CVD grown edges and resolving the ambiguity of zigzag and armchair directions using a crystallographic etching process. We employ weak antilocalization to extract the spin-orbit coupling parameters quantitatively, and report excellent reproducibility and a good match to theoretical predictions. We also confirm the influence of high pressure on the proximity effect.

HL 30.3 Wed 15:45 POT/0081

Nonlinear optical probing of local quantum geometry — •Nele Tornow[1], Paul Herrmann[1], Clemens Schneider[2], Jan Wilhelm[2], and Giancarlo Soavi[1,3] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany — [3]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

With its direct relation to many phenomena in solid matter, quantum geometry has become a concept of increasing interest in solid state physics. However, measurements of the local quantum geometry, *e.g.,* Berry curvature, has been possible to date only *via* angle-resolved photoemission spectroscopy [1]. On the other hand, in one of our recent theoretical works [2] we have shown that there is a link between linear circular dichroism and derivatives of Berry curvature in 3D crystals with preserved time-reversal symmetry (TRS).

In this presentation I will further demonstrate both, experimentally and with analytical solutions of semiconductor Bloch equations, that in a 2D semiconductor with broken TRS, the emerging second-harmonic circular dichroism can be used as a direct probe of the Berry curvature at the opposite ± K valleys, providing a new all-optical approach to access the local quantum geometry in 2D materials.

[1] Schüler, M. et al., Sci. Adv. 6, eaay2730 (2020)
[2] Soavi, G. and Wilhelm, J., arXiv:2501.03684 (2025)

15 min. break

HL 30.4 Wed 16:15 POT/0081

Proposal for Resolving Quantized Landau Orbits via Elastic XUV Scattering — •Sabrina Meyer[1], Andreas Knorr[1], Stephen Hughes[2], and Lara Greten[1,2] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

In a strong perpendicular magnetic field, a two-dimensional electron gas is quantized into discrete Landau levels. We propose a method to extract the spatial structure of Landau orbits via scattering with extreme ultraviolet radiation, whose wavelength naturally matches the Larmor radius. In a microscopic theory, we derive the far-field spectrum emitted by the optically induced current density. Contributions from Landau orbits within this spectrum are suppressed due to scattering effects imposed by the sample geometry. By normalizing against the zero-magnetic-field reference, however, we define a Landau level scattering spectrum that isolates Landau orbit information. This gives access to the probability density distributions of individual Landau level wave functions featuring radial maxima at the quantized Larmor radii.

HL 30.5 Wed 16:30 POT/0081

Berry Phase Shift in Folded Bilayer Graphene — •Hannes Kakuschke, Lina Bockhorn, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Mono- and bilayer systems of graphene have been extensively researched due to their unique magnetic und electronic transport properties. In more recent works, folded graphene [1-5] has gained interest as a platform for topological phenomena, such as zero-line modes [4]. However, these systems rely on self-assembled folded graphene, found by chance during exfoliation or induced by tearing [1-5]. Our dry-transfer approach allows us to fold graphene around hBN in a controllable manner, decoupling the overlapping graphene regions. In these samples, we observe a Berry phase shift from 2π to π near the edge of folded bilayer graphene, attributed to local strain fields and stacking shifts.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).
[4] S. J. Hong et al., 2D Materials 8, 045009 (2021).
[5] S. J. Hong et al., Phys. Rev. B 105, 205404 (2022).

HL 30.6 Wed 16:45 POT/0081

Probing spin-orbit coupling in graphene/WSe_2 heterostructures by the circular photogalvanic effect — Ernst Knöckl, •Matthias Klein, Alexander Holleitner, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

We investigate proximity-induced spin–orbit coupling (SOC) in graphene/WSe_2 heterostructures using the circular photogalvanic effect (CPGE) as a symmetry-selective and experimentally accessible probe of spin–valley-locked band textures [1]. By measuring helicity-dependent photocurrents as a function of gate voltage, excitation energy, and device geometry, we aim to disentangle Rashba and valley-Zeeman SOC contributions and to extract their magnitude and sign as a function of the graphene–WSe_2 twist angle. The observed trends in CPGE sign reversals and scaling behavior provide quantitative indications of interfacial symmetry breaking and moiré-enhanced spin–valley coupling, supported by comparison to microscopic transport models. These results are expected to establish CPGE as a promising metrological probe of proximity SOC in 2D heterostructures and to complement ongoing efforts in twist-angle-dependent spin–orbit engineering in graphene/TMD systems [2,3].

[1] Kiemle, J., et al. ACS nano 16.8, 12338-12344 (2022)
[2] Yang, H., et al. Nat. Mater. 23, 1502-1508 (2024)
[3] Zhang, Y., et al. Natur 641, 625-631 (2025)

HL 30.7 Wed 17:00 POT/0081

Study of the non-trivial spin texture in Tellurium and the consequences in charge-spin interconversion — •Andrés Martínez-García[1], Daniel Gosálvez-Martínez[1], Carlos Sabater[1], and Juan José Palacios[2] — [1]Departamento de Física and Instituto Universitario de Materiales de Alicante (IUMA), Universidad de Alicante, Alicante, Spain. — [2]Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain.

Tellurium is a chiral semiconducting material with a narrow band gap that can be synthesized with well-defined handedness in nanowires and flakes, making it an excellent platform for studying chirality-related charge-spin interconversion in nanodevices. The coupling between charge and spin degrees of freedom is closely connected to the spin texture in momentum space. In this work, we demonstrate that tellurium exhibits a nontrivial radial spin texture at the top of the valence band, where the spin polarization aligns parallel to the HK direction of the Brillouin zone, while spins in the perpendicular ZHL plane display a nontrivial winding. We investigate the electronic transport and resulting spin polarization within the Landauer transport formalism using first-principles calculations. This approach allows us to map the transport properties along each crystallographic direction and to identify correlations between the spin polarization of the induced current and the underlying momentum-space spin texture. Our results provide microscopic insight into chirality-driven spin responses in tellurium and highlight its potential for spintronic applications.

HL 31: Materials and Devices for Quantum Technology I

Time: Wednesday 15:00–16:15 Location: POT/0251

HL 31.1 Wed 15:00 POT/0251

Escaping AB caging via Floquet engineering: photo-induced long-range interference in an all-band-flat model — Aamna Ahmed, •Mónica Benito, and Beatriz Perez-Gonzalez — Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Flat-band lattices hosting compact localized states are highly sensitive to external modulation, and the tailored design of a perturbation to imprint specific features becomes relevant. Here we show that periodic driving in the high-frequency regime transforms the all-flat-band diamond chain into one featuring two tunable quasi-flat bands and a residual flat band pinned at zero quasienergy. The interplay between lattice geometry and the symmetries of the driven system gives rise to drive-induced tunneling processes that redefine the interference conditions and open a controllable route to escaping Aharonov-Bohm (AB) caging. Under driving, the diamond chain effectively acquires the geometry of a dimerized lattice, exhibiting charge oscillations between opposite boundaries. This feature can be exploited to generate two-particle entanglement that is directly accessible experimentally. The resulting drive-engineered quasi-flat bands thus provide a versatile platform for manipulating quantum correlations, revealing a direct link between spectral fine structure and dynamical entanglement.

HL 31.2 Wed 15:15 POT/0251

Floquet theory for the quantum-to-classical crossover of light-matter models — •Beatriz Perez Gonzalez[1], Sigmund Kohler[2], and Mónica Benito[1] — [1]Institute of Physics (University of Augsburg), Augsburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain

Rabi-type Hamiltonians, comprising either a time-periodic driving or a quantized electromagnetic field, have become ubiquitous across physics. Despite the well-established physics of both the semi-classical and quantum descriptions, when and how classical Floquet physics emerges from a fully quantum treatment remains the subject of active debate [1] and study [2].

We present a unified framework for the quantum-to-classical mapping, emphasizing the gauge-invariant formulation of the quantum Rabi Hamiltonian. This allows a systematic comparison of quasienergies, spectra, entanglement, and dynamics across high- and low-frequency regimes, and clarifies how Floquet frames correspond to gauge choices once photonic Fock states are interpreted as Fourier harmonics. We further assess the suitability of quantum high-frequency expansions and benchmark them against alternative methods for deriving effective Hamiltonians, including Schrieffer-Wolff transformations and projector-based approaches.

[1] Phys. Rev. Lett. 129, 183603 (2022); Phys. Rev. Research 2, 033033 (2020); [2] B. Perez-Gonzalez et al., Quantum 9, 1633 (2025); Comm. Phys. 7, 419 (2024)

HL 31.3 Wed 15:30 POT/0251

Understanding optically detected magnetic resonance (ODMR) of InSi-Sii-defects — •Kevin Lauer[1,2], Bernd Hähnlein[1], Mario Bähr[1], Kai Kühnlenz[1], Philipp Kellner[1], Dirk Schulze[2], Stefan Krischok[2], Alexander Rolapp[3], Christian Möller[1], and Thomas Ortlepp[1] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — [2]Technische Universität Ilmenau, Institut für Physik, Weimarer Str. 32, 98693 Ilmenau, Germany — [3]IMMS Institut für Mikroelektronik- und Mechatronik-Systeme gGmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Defects from the acceptor-interstitial silicon (ASi-Sii)-defect category were found to be promising candidates for qubits in silicon-based quantum technology [1]. To further explore their qubit properties optically detected magnetic resonance (ODMR) measurements are carried out on quenched indium-doped silicon samples featuring InSi-Sii-defects. Depending on the antenna design (omega or rod) four different ODMR signals are found in the spectra. An approach to understand these spectra in frame of a triplet system formed by two holes at the InSi-Sii-defect will be discussed. On that basis possible electronic level schemes are proposed.

[1] K. Lauer et al., 'Examining the properties of the ASi-Sii-defects for their potential as qubits', presented at the GADEST but unpublished, Bad Schandau: ResearchGate, May 2024. doi: 10.13140/RG.2.2.18793.51048.

HL 31.4 Wed 15:45 POT/0251

Time-bin encoded quantum key distribution over 120 km with a telecom quantum dot source — •Jingzhong Yang[1], Jipeng Wang[1], Joscha Hanel[1], Zenghui Jiang[1], Raphael Joos[2], Michael Jetter[2], Eddy. Patrick Rugeramigabo[1], Simone. Luca Portalupi[2], Peter Michler[2], Xiao-Yu Cao[3], Hua-Lei Yin[3,4], Shan Lei[5], Jingzhong Yang[1], Michael Zopf[1], and Fei Ding[1] — [1]Leibniz University of Hannover, Hannover, Germany — [2]University of Stuttgart, Stuttgart, Germany — [3]Nanjing University, Nanjing, China — [4]Renmin University of China, Beijing, China — [5]Anhui University, Hefei, China

Quantum key distribution (QKD) with deterministic single photon sources has been demonstrated over intercity fiber and free-space channels, but mainly on polarization encoding schemes. In contrast, time-bin encoding offers inherent robustness and has been widely adopted in mature QKD systems using weak coherent laser pulses.

In this work, we presents the first demonstration of the time-bin encoded quantum key distribution (QKD) using the telecom single photons from a quantum dot. A maximum tolerable transmission distance of 127 km is identified as the system error ratio approaches the security threshold. The result demonstrates the feasibility of realizing robust and scalable quantum communication network based on solid-state single-photon technology.

HL 31.5 Wed 16:00 POT/0251

high-efficiency photonic interfaces for VV centres in silicon carbide — •Nien-Hsuan Lee[1,2], Jonas Schmid[1,2], Berke Demiralp[3], Felix David[1], Kevin Menguelti[3], Stephan Kucera[1], Eva Weig[3,4,5], and Florian Kaiser[1,2] — [1]Luxembourg Institute of Science and Technology, Belval, Luxembourg — [2]University of Luxembourg, Belval, Luxembourg — [3]Technical University of Munich, Garching, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany — [5]TUM Center for Quantum Engineering, Garching, Germany

In this work, we present a systematic investigation of etching processes aimed at optimising photonic structures for VV centres in bulk SiC. A wide range of fabrication parameters is explored, including metallic and non-metallic etch masks, plasma chemistries, and etching strategies to reduce surface and sidewall roughness while improving reproducibility. Structural and optical characterisation of the resulting waveguides enables identification of key loss mechanisms and the critical parameters governing high-efficiency photon transmission. Building on these process developments, we demonstrate a new generation of free-standing SiC waveguides with high wafer-scale uniformity and excellent reproducibility, enabling very high coupling efficiencies. Furthermore, we introduce a nanocone photonic structure in SiC, which simulations indicate can achieve more than a ten-fold enhancement in photon collection efficiency compared with unstructured bulk SiC. These results provide a scalable and reproducible photonic platform for wafer-scale integration of SiC colour centres for quantum communication.

HL 32: 2D Materials 2 (joint session DS/HL)

Time: Wednesday 15:00–17:30 Location: REC/C213

HL 32.1 Wed 15:00 REC/C213

Engineering at the Thinnest Scale: Insights into the Stability of 2D GaN on Liquid Metal Catalysts — •Tomoko Yokaichiya, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Hexagonal GaN (h-GaN), theorized to be metastable when confined to only a few nanometers, stands out as a promising wide-bandgap semiconductor for next-generation nanoelectronics. Although early studies report that h-GaN can be synthesized using e.g. liquid metal catalysts, its definitive experimental identification is challenging. This difficulty arises from a structural ambiguity due to possible defects, multilayer-stacking variations, and competing polymorphs of h-GaN's characteristic honeycomb structure, as predicted by pioneering, yet simplified electronic-structure studies. In this work, we use density functional theory alongside large-scale atomistic simulations based on machine-learned interatomic potentials to re-assess the stability of h-GaN at finite temperatures and in the presence of a liquid metal substrate. We systematically investigate the structural and electronic properties of h-GaN, examining how they evolve with layer thickness and possible structural variations. Furthermore, we analyze its thermodynamic competition with bulk wurtzite GaN and alternative thin-film polymorphs, including a previously suggested haeckelite phase. Our results reveal that h-GaN exists within a delicate stability window. Based on these insights, we propose key signatures to guide experimental detection and outline whether h-GaN may become synthesizable as a feasible 2D semiconductor.

HL 32.2 Wed 15:15 REC/C213

Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ — •Timon Mosko[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Safarik University in Kosice, Park Angelinum 9, 04001 Kosice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Kosice, Slovakia

The monolayer α-$TaSi_2N_4$ belongs to the recently discovered MA_2Z_4 family of two-dimensional intercalated materials, exhibiting wide range of physical properties, including semiconducting, metallic, topological, and superconducting behavior. Members of this group, such as $MoSi_2N_4$, WSi_2N_4 have already been successfully synthesized, highlighting the structural and electronic tunability of the inspected group of materials. We investigated the superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ using a combination of ab initio and effective model approaches. The phonon-mediated superconductivity is examined through first-principles calculations, an effective tight-binding Hamiltonian in Wannier basis and further analyzed within the Migda-Eliashberg theory of superconductivity. Our results reveal that α-$TaSi_2N_4$ is an anisotropic two-band superconductor. Additionally, we study the dielectric response via electric susceptibility using linear response theory within the RPA, combining Green's function formalism with tight-binding modeling.

This work was supported by the Slovak Academy of Sciences project IMPULZ IM-2021-42, and by the Ministry of Education, Research, Development and Youth of the Slovak Republic, provided under Grant No. VEGA 1/0104/25.

HL 32.3 Wed 15:30 REC/C213

Probing the Quantum Spin Hall State in Atomic Monolayers via NanoARPES — •Cedric Schmitt[1,2], Lukas Gehrig[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Matthew Watson[3],

Jörg Schäfer[1,2], Simon Moser[1,2,4], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Diamond Light Source, UK — [4]AG Oberflächen, Ruhr-Universität Bochum

Our recently discovered quantum spin Hall insulator indenene [1], a triangular monolayer of indium on SiC(0001), exhibits a 120 meV gap and monodomain growth on the μm scale. To verify its topological nature, we use circular dichroism in ARPES as a bulk-sensitive probe of orbital angular momentum (OAM) linked to its Berry curvature [2]. Due to SiC's stepped morphology, stacking-dependent OAM cancellation complicates microARPES. We overcome this challenge using nanoARPES with sub-600 nm resolution, resolving OAM asymmetry at individual terraces of SiC. Our study establishes dichroism as a robust spectroscopic tool for topological classification within a single SiC terrace.

[1] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)
[2] J. Erhardt et al. Phys. Rev. Lett. 132, 196401 (2024)

HL 32.4 Wed 15:45 REC/C213

Physical Properties of $Ti_3C_2Cl_2$ MXenes — •Moritz Vanselow[1], Maksim Riabov[2], Thierry Ouisse[2], Hanna Pazniak[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

Hydrophobic $Ti_3C_2Cl_2$ MXenes are synthesized by Lewis acid molten-salt etching of $Ti_3C_2Cl_2$ followed by delamination process[1] and subsequently deposited from acetonitrile suspension ($\sim$ 0.1 mg/mL) on $Si(100)/SiO_2$ substrates. Using in-situ mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum, we show that $Ti_3C_2Cl_2$ exhibits enhanced thermal robustness up to 900°C as compared to conventional mixed-terminated $Ti_3C_2T_x$ MXenes with $T_x = -F, = O,$ and $-OH$. Complementary ex situ XRD and XPS confirm the absence of intercalated water and uniform $-Cl$ terminations, resulting in sharp and intense (00l) peaks with $c = 2.223 \pm 0.015$ nm and reflecting its high degree of structural order. Low-temperature specific heat measurements reveal distinct phonon signatures expected for the two-dimensional $Ti_3C_2Cl_2$. We determined the Debye temperature to 548 K in a temperature interval 20–50 K consistent with DFT model calculations[2] and a Sommerfeld constant of $\gamma = 19.2\,\mathrm{mJ\,mol^{-1}\,K^{-2}}$. This work is supported by ANR-23-CE09-0031-01 and DFG ID 530103526.

[1] T. Zhang et al., Chem. Mater. 36, 1998 (2024). [2] M. Riabov, M. Vanselow, et al., npj 2D Materials & Applications 2025, accepted

HL 32.5 Wed 16:00 REC/C213

Phase field crystal model of out-of-plane deformations in thin crystalline sheets induced by thermal expansion — •Emma Radice[1], Marco Salvalaglio[1,2], and Axel Voigt[1] — [1]Institut für Wissenschaftliches Rechnen, Technische Universität Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Thin, flexible crystalline sheets exhibit unique elastic properties due to their ability to undergo out-of-plane deformations.Understanding this behavior requires a description that couples in-plane elasticity, out-of-plane bending and the presence of defects. We develop a mesoscale description for these systems by extending the Phase-Field Crystal (PFC) model. PFC model describes crystal structures at diffusive timescales through a periodic, microscopic density field and it allows one to incorporate both elasticity and topological defects into a continuum description. Our extension permits a spatially varying equilibrium lattice spacing, enabling the representation of localized lattice eigenstrain to mimick thermal effects or lattice mismatch in heterostructures. We validate the extended model against analytical predictions from the Föppl von Kármán equations for uniaxial compression and from Eshelby's inclusion problem. Using this validated framework, we then study how locally induced compressive stresses drive out-of-plane deformation (buckling) in the sheets. Our approach, implemented via a Fourier pseudo-spectral method, exploits the PFC model's natural ability to capture the complex, coupled interactions among elasticity, out-of-plane bending and defect dynamics.

15 min. break

HL 32.6 Wed 16:30 REC/C213

Magnetotransport in Z-Folded ABC-Stacked Trilayer Graphene Structures — •Maximilian Mischke, Lina Bockhorn, Sofiya Lazareva, and Rolf Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Folded graphene (multi)layers promise to contain rich and interesting physics [1-3], so we produced a sample to investigate the influence of such a fold on magnetotransport properties of graphene. The measurements were carried out in a 4He cryostate at 1.4 K while the samples' carrier concentration was controlled via a global backgate. The sample itself consists of a z-folded ABC-trilayer graphene partially encapsulated in hBN with electrical contacts that allow for measurements in the unfolded region as well as through the fold. We observed filling factors that are unexpected for ABC-trilayer graphene. The untypical transport behaviour can be explained by angle dependend interlayer coupling and screening effects in the z-fold.

[1] S. J. Hong et al, Phys Rev B 105, 205404 (2022)
[2] H. Schmidt et al, Nature Communications 5(1), 5742 (2014)
[3] Y. Liu et al, Phys Rev B 92, 235438 (2015)

HL 32.7 Wed 16:45 REC/C213

Quantum dots in proximitized BLG/TMD heterostructures — •Ching-Hung Chiu and Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

Bilayer graphene (BLG) has attracted attention recently due to the possibility of inducing layer-selective Spin-orbit coupling (SOC) by proximitizing with transition metal dichalcogenides (TMDs) [1,2]. Simultaneously, the gate-tunable band gap in BLG enables electrostatic confinement of charge carriers into gate-defined quantum point contacts and quantum dots [3,4]. Here, we theoretically investigate the interplay of proximity effects and confinement by studying confined quantum states in proximitized BLG/TMD quantum dots. We calculate the states' properties, such as their splittings and spin polarisation, as a function of SOC coupling parameters and the dot's size and shape. Our studies go alongside experimental realisations of confinement in BLG/TMD heterostructures [5,6] and pave the way for using and controlling the dot's spin and valley states as qubits.

[1] K. Zollner and J. Fabian, Phys. Rev. B 104, 075126 (2021)
[2] A. M. Seiler et al., 2025 2D Mater. 12 035009
[3] H. Overweg et al,, Phys. Rev. Lett. 121, 257702 (2018)
[4] S. Möller et al., Phys. Rev. Lett. 127, 256802 (2021)
[5] J. D. Gerber et al., Nano Lett. 2025, 25, 33, 12480-12486
[6] H. Dulisch et al., Nano Lett. 2025, 25, 26, 10549-10555

HL 32.8 Wed 17:00 REC/C213

Influence of Polymethyl Methacrylate molecular weight on Graphene transfer and its intrinsic properties — •Monika Choudhary[1], Rasuole Lukose[1], Moriom Akter[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]Leibniz-Institut für Innovative Mikroelektronik (IHP), Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

Polymethyl methacrylate (PMMA)-assisted wet transfer is widely used for integrating large-scale graphene grown on Ge(100)/Si substrates via chemical vapor deposition onto insulating SiO2/Si substrates[1,2]. However, the influence of PMMA molecular weight (MW) on properties of transferred graphene is insufficiently quantified. To address this, we investigate graphene transferred using low (50K), medium (600K), and high (950K) MW PMMA to isolate how polymer chain length governs film integrity and contamination. Characterization by atomic force microscopy (AFM), and spatially resolved X-ray photoelectron spectroscopy (XPS) reveals reduced contamination and smoother topography for graphene with 600K transfers. Additionally, micro-Raman spectroscopy demonstrates strain-free graphene with reduced doping and a 2D peak full width at half maximum (FWHM) of 35.53 cm-1 consistent with as-grown values. 1. Akhtar F., et al. ACS Appl. Mater. Interfaces 15 (2023). 2. Lukose R., et al. Scientific Reports 11 (2021). Acknowledgement: This research was funded by the European Union*s Horizon Europe research and innovation programme under grant agreement No 101120938 (GATEPOST).

HL 32.9 Wed 17:15 REC/C213

High-performance graphene field-effect transistors on cyclic olefin copolymer substrates for advanced sensor applications — •Hamid Reza Rasouli[1], Begimai Adilbekova[1], Ghazaleh Eshaghi[1], Axel Printschler[1], David Kaiser[1], Marco Reinhard[2], Alexander Rolapp[2], Tom Reinhold[2], Uwe Hübner[3], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]IMMS Institut für Mikroelektronik- und

Mechatronik-Systeme gemeinnützige GmbH (IMMS GmbH), 99099 Erfurt, Germany — [3]Leibniz Institute of Photonic Technology, Albert-Einstein-Straße 9, 07745 Jena, Germany

While graphene field-effect transistors (GFETs) are highly attractive for liquid-phase sensing, their performance on SiO2/Si substrates is compromised by oxide-induced charge trapping, leading to pronounced hysteresis and reduced stability. We present arrays of GFETs microfabricated on cyclic olefin copolymer (COC) substrates, which passivate SiO2 providing a low-trap and chemically inert platform in combination with flatness. GFET devices on COC demonstrate remarkably improved Dirac point stability, negligible hysteresis even in low-ionic strength buffers, and reproducibility across the arrays. For their functionalization, we employ an ultrathin carbon nanomembrane (CNM) that enables robust immobilization of various capture molecules while preserving graphene's transport properties. The CNM/GFET/COC architecture provides stable liquid-phase operation highlighting its strong potential for scalable and advanced sensor applications.

HL 33: Nitrides I – Growth and fabrication

Time: Wednesday 16:30–17:45 Location: POT/0006

HL 33.1 Wed 16:30 POT/0006

Homoepitaxial growth of AlN by plasma-assisted molecular beam epitaxy — •Xin Du, Hossein Yazdani, and Yongjin Cho — Paul-Drude-Institut für Festkörperelektronik (PDI), Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

Wurtzite AlN can be considered an electrical insulator because of its ultrawide bandgap of 6.2 eV. However, it can become electrically active as either n-type or p-type through direct chemical doping or polarization doping when alloyed with the other group-III cations. This broad tunability in electrical conductivity, combined with its high thermal conductivity of about 340 W/m·K, makes AlN highly attractive for power electronics and deep-UV optoelectronic devices. Interest in AlN has considerably increased with the recent development of high-quality AlN bulk substrates with dislocation densities below 10^4 cm^{-2}. To fully leverage the high structural quality of these substrates in subsequent epitaxial layers, the native oxide must be removed before growth. Although Al-assisted deoxidation of AlN substrates has recently been shown to be effective for MBE growth, achieving consistently complete oxide removal and subsequently high-quality AlN homoepitaxy remains challenging. In this talk, we show how various cleaning methods and MBE growth conditions influence AlN homoepitaxy. This work serves as a seeding study at PDI for future investigations aimed at achieving reliable doping control in AlN with minimized compensating defects.

HL 33.2 Wed 16:45 POT/0006

Phase transition regions of epitaxially sputtered TiAlN layers on TiN and AlN buffer layers — •Emine Kaynar, Florian Hörich, Jürgen Bläsing, Fabian Grossmann, Usha Velpuri, Armin Dadgar, André Strittmatter, and Arne Busse — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

For manufacturing vertical GaN-based power devices on Si substrates, it is advantageous to replace insulating AlN/AlGaN layers at the Si interface. AlN/AlGaN layers are currently required to ensure high-quality GaN on Si. TiAlN alloys offer a tunable bandgap from metallic conduction up to 6 eV and thermal robustness, making them promising alternatives to insulating Al(Ga)N buffers when epitaxial growth on Si is feasible. In this work, TiAlN layers were epitaxially grown on n-type Si (111) using TiN and AlN buffers prepared by a two-step sputtering process at growth temperatures below 900 °C. Highly crystalline cubic TiN (ω-FWHM ~ 0.3°, RMS $<$ 1 nm) served as a conductive template. By tuning the power ratio between Ti and Al targets, Al content was systematically controlled, enabling direct mapping of the cubic-wurtzite transition. On TiN buffers, cubic TiAlN remained stable up to x ~ 0.4. On wurtzite AlN buffers, the opposite transition from wurtzite to cubic occurred as Ti incorporation increased. For all AlN-buffered samples, ω-FWHM stayed below 1° and RMS roughness remained $<$ 5 nm. These results demonstrate precise phase control and high crystalline quality, positioning TiAlN as a strong candidate for conductive buffer layers in vertical GaN-on-Si device architectures.

HL 33.3 Wed 17:00 POT/0006

Epitaxial Growth of ZrN on Si(111) — •Muthukani Kathiresan, Usha Velpuri, Arne Busse, Florian Hörich, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

Transition metal nitrides can add new functionalities to GaN devices. These range from conducting buffer layers for the growth of vertical GaN devices on Si, as template for the growth of N-polar GaN up to enhanced piezo- and ferroelectric properties when alloyed with AlN. Transition-metal nitrides (TMNs) such as ZrN, HfN, TiN and ScN crystallize in the rock-salt structure and exhibit metallic conductivity except for ScN which is semiconducting. For nitride growth, ZrN is particularly attractive due to its favorable lattice relationship, exhibiting an in-plane mismatch of only 1.35% between ZrN (111) and GaN (0001). Additionally, ZrN layers can be deposited by sputtering, whereas layer growth by MOVPE suffers from the low-vapor pressure of available precursors.In this work, we present recent progress in the sputter epitaxy of ZrN on Si (111). For 100-nm-thick films grown at 900 °C in N2/NH3, we achieved an ω-FWHM of 0.5°. Introducing NH3 promoted a transition from a columnar grain structure to a compact, two-dimensional morphology, with a surface roughness of 1.7 nm. The thermal stability of these layers was assessed through annealing at 1100 °C under NH3, which led to reduced film density by void formations, revealed by X-ray reflectivity (XRR) measurements and scanning electron microscopy (SEM).

HL 33.4 Wed 17:15 POT/0006

In-situ fabrication of $In_{0.3}Ga_{0.7}N$ pseudo-substrates on GaN (0001) templates via a three-step protocol in plasma-assisted molecular beam epitaxy — •Huaide Zhang, Aidan Campbell, Jingxuan Kang, Jonas Lähnemann, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117, Berlin, Germany

The considerable lattice mismatch between GaN and InN introduces significant strain into (In,Ga)N epitaxial layers grown on GaN templates. This strain impedes the incorporation of In and induces a strong piezoelectric field in (In,Ga)N/GaN quantum wells, which diminishes the internal quantum efficiency. Furthermore, the accumulated strain can prompt plastic relaxation of the lattice, generating additional threading dislocations. The high In content required for (In,Ga)N-based light-emitting diodes (LEDs) operating in the amber/red spectral range necessitates, hence, a substrate with an adjusted lattice constant. In this work, we present a three-step growth method for fabricating a highly relaxed $In_{0.3}Ga_{0.7}N$ pseudo-substrate directly on GaN(0001) templates which is conducted entirely within a plasma-assisted molecular beam epitaxy system. In contrast to other approaches, our method does not require any ex-situ patterning, providing thus advantages in terms of scalability and cost. The resulting structure demonstrates superior characteristics in key properties, including In content, degree of strain relaxation, and surface smoothness compared to existing alternatives.

HL 33.5 Wed 17:30 POT/0006

Influence of A-Site Cations on Structure, Defect Density and Photoactivity of Tantalum-Based Perovskite Oxynitride Photoelectrodes — •Gabriel Grötzner[1,2], Aleksandr Kochergov[1,2], Oliver Brune[1,2], Laura I. Wagner[1,2], Saswati Santra[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

Perovskite oxynitrides are emerging materials for photoelectrochemical (PEC) water splitting, yet the influence of the A-site cation on their material properties remains poorly understood. Here, we investigate a series of $ATaON_2$ thin films (A = La, Ce, Pr, Nd, Gd, ordered by decreasing ionic radius) to elucidate the role of the A-site cation

on structural, optoelectronic, and PEC properties. X-ray diffraction analysis reveals a systematic lattice contraction with decreasing ionic radius of the A-site cation. This structural change is accompanied by an increase in optical band gap from 1.8 eV to 2.2 eV and a reduction in sub-bandgap absorption, indicating lower defect densities for smaller A-site cations. Electrical measurements show reduced conductivity for $GdTaON_2$ compared to $LaTaON_2$, consistent with defect suppression. By changing the A-site cation from La to Gd, the photocurrent density in PEC measurements doubles, despite an increase in optical band gap, which indicates the beneficial impact of reduced defect-mediated recombination. These insights offer design principles for defect and band-structure engineering in perovskite oxynitride photoanodes.

HL 34: Quantum Dots and Wires: Telecom Wavelength

Time: Wednesday 16:30–17:45 Location: POT/0051

HL 34.1 Wed 16:30 POT/0051

All-photonic quantum teleportation at telecom wavelength with frequency converted photons from remote quantum dots — •Tim Strobel[1], Michal Vyvlecka[1], Ilenia Neureuther[1], Tobias Bauer[2], Marlon Schäfer[2], Stefan Kazmaier[1], Nand Lal Sharma[3], Raphael Joos[1], Jonas H. Weber[1], Cornelius Nawrath[1], Weijie Nie[3], Ghata Bhayani[3], Caspar Hopfmann[3], Christoph Becher[2], Peter Michler[1], and Simone Luca Portalupi[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Dresden, Germany

A future terrestrial quantum internet relies on distant quantum network nodes connected via optical fiber channels. In this context, semiconductor quantum dots (QDs) are promising sources of quantum light. Here, we report on an all-photonic quantum teleportation experiment with photons from remote QDs emitting at ca. 780 nm. The polarization state of a single photon emitted by one QD is prepared and interfaced with one photon of an entangled pair from a second QD in a Bell state measurement. This process teleports the polarization state onto the second photon of the entangled pair. Polarization-preserving quantum frequency converters eliminate the frequency mismatch between photons, allowing for interference at telecom wavelengths. Teleportation succeeds with post-selected fidelities up to 0.721(33).

HL 34.2 Wed 16:45 POT/0051

Telecom C-band Quantum Dots Coupled to Gaussian-shaped Microlens Cavities — •Michelle Pfahl[1], Raphael Joos[1], Lena Engel[1], Johannes Michl[2], Katharina Dahler[1], Ponraj Vijayan[1], Tobias Huber-Loyola[2], Michael Jetter[1], Simone L. Portalupi[1], Sven Höfling[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Julius-Maximilians-Universität Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg

Single-photon sources emitting in the telecom C-band are a key resource for applications in quantum communication and quantum cryptography, as they enable long-distance quantum networks. Semiconductor quantum dots (QDs) are particularly well suited for this since they have a high quality optical emission and can achieve high efficiency when coupled to microcavities. Here, we investigate telecom C-band InAs QDs, which are embedded in a resonator made of distributed Bragg reflectors (DBRs), with the upper dielectric DBR being shaped into Gaussian lenses using an etching process. This structure promises Purcell enhancement, which reduces the decay time of the QDs and enables efficient collection of the emitted photons. We investigate the optical modes of the resonators by an in-depth characterization of microlenses with different design parameters. Furthermore, the quantum-optical properties of the QDs coupled to cavities are analyzed by means of autocorrelation and decay time measurements.

HL 34.3 Wed 17:00 POT/0051

InGaAs/GaAs preparation at 1.55 micrometer telecom wavelengths — •Juwana Jose, André Strittmatter, Armin Dadgar, Jürgen Bläsing, and Usha Velpuri — Otto von guericke university, Magdeburg, Germany

Quantum key distribution is a secure way of generating and sharing encryption keys using photons. Single photons as qubits for key generation is an efficient method of secure data transmission. It guarantees absolute eavesdropping detection since it is impossible to copy a quantum state. Qubit transmission at telecom wavelengths of 1.55 micrometer using InGaAs quantum dots on GaAs substrates is a challenge. We explore the conventional Stranski-Krastanow growth mode to shift the wavelengths far beyond the spectral 1.3-1.4 *m region. Photoluminescence experiments on high-density QD ensembles show remarkable intensities in a wavelength range of 1.5-1.6 micrometer at room-temperature. This luminescence shifts by xx nm into the blue upon cooling down to 15 K. By tailoring the thickness of the initial InGaAs deposition to the 2D/3D transition region low QD densities of 108 cm-2 and below are achieved. Single photon emission experiments will be conducted after preparation of individual QD emitters.

HL 34.4 Wed 17:15 POT/0051

Integration of telecom C-band quantum dot-based single-photon emitters onto silicon photonic platform using micro-transfer printing — •Simon Oberle[1], Ponraj Vijayan[1], Alessandro Buzzi[2], Hugo Larocque[2], Michael Jetter[1], Simone Luca Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), University of Stuttgart — [2]Research Laboratory of Electronics (RLE), Massachusetts Institute of Technology

Silicon photonics for telecommunications applications has garnered much attention recently. The optical transparency and the large refractive index contrast of silicon at telecommunication wavelengths allow the implementation of high-density photonic integrated circuits. One disadvantage of silicon photonics is the lack of mature deterministic light sources. One potential solution is the integration of III-V material, which offers outstanding optical emission properties, on a silicon platform. The direct growth of III-V materials on silicon the most scalable and therefore desired approach. However, it is challenging because of the material polarity difference and the lattice mismatch between GaAs and silicon. An alternative approach is the hybrid integration of III-V structures using micro-transfer printing, which enables integration of prefabricated devices onto silicon. Our group has previously developed telecom C-band emitting InAs quantum dots grown on InGaAs. Here, we report our approach to designing and fabricating structures for the hybrid integration of these QDs onto a silicon platform using micro-transfer printing.

HL 34.5 Wed 17:30 POT/0051

Automated optical imaging for telecom Quantum Dot deterministic fabrication — •Eden Arbel[1], Lukas Wagner[1], Peter Gierss[1,2], Ponraj Vijayan[1], Michal Vyvlecka[1], Michael Jetter[1], Simone L. Portalupi[1], 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, Allmandring 3, 70569 Stuttgart, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig

Semiconductor quantum dots (QDs) are promising sources of single- and entangled-photon pairs. Due to its low absorption in silica fibers, operation in the telecom C-band (1530-1565nm) is desired. Integrating these QDs into Circular Bragg Grating cavities (CBGs) enhances extraction efficiency and enables Purcell enhancement. Our method employs wide-field imaging for deterministic preselection of QDs for subsequent CBG fabrication. The QD positions are referenced using e-beam-written markers. Smart preselection of suitable candidates, embedded in an automated setup, promises higher yield and efficiency, with the potential for AI integration. We demonstrate that deterministically processed CBGs exhibit significant improvements in brightness and enhance the decay time of the two-level state. With higher throughput and continually improving quality of telecom QD samples, this approach will enable to provide single-photon sources tailored to specific needs of various applications, such as quantum memories or long-distance quantum communication.

HL 35: Optical Properties II

Time: Wednesday 16:30–19:00 Location: POT/0251

HL 35.1 Wed 16:30 POT/0251

Polarization-Angle-Resolved Raman Spectroscopy for Reliable Raman Tensor Analysis — •Hans Tornatzky[1], Jonas Rose[1], Luca Choi[2], Moritz Meissner[1], Zbigniew Galazka[3], and Markus R. Wagner[1,2] — [1]Paul Drude Institut — [2]Technische Universität Berlin — [3]Institut für Kristallzüchtung

Phonons are fundamental to materials, shaping the physical properties that underlie device functionality. Accurate knowledge of their quantitative description, specifically the Raman tensor, is essential for a detailed understanding of materials and for reliable modeling and optimization of structures and devices.

This talk presents state-of-the-art approaches for determining relative Raman tensor elements using polarization-angle-resolved Raman (PARRS) spectroscopy, alongside discussion of major challenges and sources of error encountered in the process. We also introduce a newly developed fitting procedure that enables robust disentanglement of strongly overlapping signals arising from different modes, permitting precise extraction of their characteristics – energy, FWHM, symmetry, and tensor elements – with enhanced reproducibility.

These techniques are demonstrated across several materials recently studied by our group, including rutile GeO_2, Ga_2O_3, and $LaInO_3$.

HL 35.2 Wed 16:45 POT/0251

Characterization of Exciton-exciton entanglement in different phases: A many-body investigation in low dimensions — •Fangzhou Zhao[1], Carlos Mejuto-Zaera[2], Vojtech Vlcek[3], and Angel Rubio[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Laboratoire de Physique Théorique, LPT, CNRS, Toulouse, France — [3]UCSB, Santa Barbara, USA

There have been emerging experimental investigations on exciton-exciton correlations, especially in moiré superlattices. However, theoretical understanding of exciton-exciton interactions - which requires an accurate treatment of four-point Green's functions and the validity of a bosonic description of excitons- remains relatively underdeveloped. We construct an exactly solvable one-dimensional model to investigate exciton-exciton correlations and entanglement using many-body exact techniques. We identify phase boundaries separating excitonic phases with different degrees of binding, and extrapolate the data to the thermodynamic limit to infer properties in large systems. We also apply a wavefunction projection technique to characterize the strength of entanglement between excitons, as well as the strength of entanglement between the electron and hole inside an exciton. Our results show that, over a broad parameter range, excitonic correlations remain weak, validating the applicability of many-body perturbation theory in most cases. We also explored the quantum confinement effect of multi-exciton state in 1D systems and uncovered the conditions under which the confinement effects emerge.

HL 35.3 Wed 17:00 POT/0251

Excited-state trions in a quantum well — Sourabh Jain[1], Mikhail Glazov[2], and •Ashish Arora[1] — [1]Indian Institute of Science Education and Research, Pune 411008 India — [2]St. Petersburg, Russia

Recently, excited-states of trions were discovered in a layered semiconductor raising strong interest in many-body physics of Coulomb-bound quasiparticles in solids [1]. Here, we report on the observation of an excited 2s state of a trion in a GaAs quantum well (QW) using magneto-optical Kerr effect (MOKE) spectroscopy under out-of-plane magnetic fields up to 6 T [2]. This resonance appears slightly below the 2s exciton in energy. Strikingly, the 2s trion is found to be bound only for magnetic fields larger than 1 T. The signature of the 2s trion is absent in the magneto-reflectance spectra, while it is detectable in the MOKE spectra signifying the importance of the powerful technique. Similar to the 1s states, the 2s trion shows an opposite degree of magnetic-field-induced polarization compared to its exciton counterpart, in agreement with our theoretical calculations. This transfer of oscillator strength between the complexes establishes an optical fingerprint of the 2s excited trion. Our work addresses a four-decade old problem of excited-state trions in a quantum well, and opens scope for further investigations of many-body physics in solids. [1] Phys. Rev. Lett. 123, 167401 (2019) [2] Phys. Rev. Lett. 134, 246902 (2025)

HL 35.4 Wed 17:15 POT/0251

Directional lasing and optical coupling in indium phosphide nanowires — •Lukas Raam Jäger[1], Wei Wen Wong[2], Hark Hoe Tan[2], and Carsten Ronning[1] — [1]Friedrich-Schiller-Universität Jena, Fürstengraben 1, 07743 Jena, Germany — [2]The Australian National University, Canberra ACT 2600, Australia

Indium phosphide (InP) nanowires (NWs) are promising nanoscale light sources due to their strong optical confinement and compatibility with selective-area epitaxy. We investigate optical coupling in vertically standing lasing InP NWs using finite-difference time-domain simulations and angle-resolved photoluminescence. Single NWs lase in the TE01 mode for diameters above about 250 nm and exhibit far-field patterns shaped by interference of emission from the top and bottom facets. Coupled NW structures enable controlled emission engineering. In NW pairs, coupling splits the TE01 mode into two hybrid modes with orthogonal directional lobes, in good agreement with experiment. Mode selection is highly sensitive to subtle geometric differences, while asymmetric pumping has negligible effect. Extending this concept to arrays of NW pairs shows that array-level interference can further narrow the emission lobes. Triplet NW structures exhibit three distinct hybrid modes with characteristic far-field patterns. These results demonstrate designable directional nanoscale emitters based on coupled NW lasers.

HL 35.5 Wed 17:30 POT/0251

Optical emission of monolayer-hybridized nanowire lasers — •Moritz Willems, Edwin Eobaldt, Alexander Zaunick, Aurelia Eberhard, Lukas Jäger, Xiao Chen, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Semiconductor Nanowires have attracted substantial scientific interest as foundation for nanoscale coherent light sources and all-optical circuits, based on to their remarkable waveguide properties and their intrinsic ability to lase. 2D-Materials offer a functional environment that enables influencing the lasing characteristics, including emission wavelength and lasing threshold, of ZnO nanowires. These hybrid structures thus allow for electrical and optical charge and energy transfer. Deterministic nanowire integration is achieved through stage-assisted transfer using PDMS and tip-assisted nanomanipulation. Comparative micro-photoluminescence measurements are used to investigate how the 2D-materials influence and modify the lasing behaviour of individual nanowires.

HL 35.6 Wed 17:45 POT/0251

Bandgap and exciton engineering in two-dimensional transition $Mo_{1-x}W_xSe_2$ alloys for next-generation photonics. — •Muhammad Hussain[1], Omid Ghaebi[1], Mohammad Monfared[2], Marco Gruenewald[1], Umer Ahsan[3], Fedor Lipilin[3], Jan Luxa[3], Zdenek Sofer[3], Ulf Peschel[2,4], and Giancarlo Soavi[1,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany. — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [4]Abbe Center of Photonics, Friedrich Schiller University Jena, Germany

Alloys of 2D transition metal dichalcogenides (TMDs), provide a unique platform for bandgap engineering at the atomic scale. In this work, we investigate the nonlinear optical response of $Mo_{1-x}W_xSe_2$ alloys focusing in particular on second harmonic generation (SHG) and two-photon photoluminescence (TP-PL) [1]. We find that alloyed TMDs exhibit enhanced nonlinearities compared to their pristine counterparts. By combining SHG and TP-PL and the respective optical selection rules, we are able to extract the energy difference between 1s and 2p exciton states in samples of different alloy composition. By doing this, we find that the exciton binding energy in such alloys varies with the W composition (x). This can be used as a knob to tune not only the optical bandgap, but also the exciton binding energy by changing the alloy composition.

[1] M. Hussain, et al. Adv. Opt. Mater. 13, 01000 (2025).

15 min. break

HL 35.7 Wed 18:15 POT/0251

Photoluminescence of single color centers in hBN below the diffraction limit — •Iris Niehues[1], Daniel Wigger[2], Korbinian Kaltenecker[3], Annika Klein-Hitpass[1], Johannes Binder[4], Andrzej Wysmołek[4], and Rainer Hillenbrand[5] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany — [3]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [4]Faculty of Physics, University of Warsaw, Poland — [5]CIC nanoGUNE BRTA, Spain

Color Centers in hexagonal boron nitride (hBN) are promising quantum light sources due to their stable single-photon emission at room temperature. Using a scattering-type near-field optical microscope, we investigate photoluminescence (PL) properties of hBN grown via metalorganic vapor phase epitaxy. Our experiments employ the microscope in tapping mode to detect PL signals influenced by the metallic AFM tip. We demonstrate near-field optical excitation and emission via the tip's nanofocus, creating a sub-diffraction limited tip-enhanced (TE)PL hotspot [1]. Additionally, an "arc" forms around the emitter, explained by constructive interference between direct beams between the optics and the emitter and indirect beams scattered from the tip. This tip-assisted (TA)PL method can be used to map in-plane dipole orientations of hBN color centers at the nanoscale.

[1] I. Niehues et al., Nanophotonics 14(3), 335-342 (2025)

HL 35.8 Wed 18:30 POT/0251

Role of lattice temperature for the optical properties of boron nitride — •Peter Kratzer[1] and Andre Schleife[2] — [1]Faculty of Physics, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, USA

We carried out a computational study of boron nitride both in its cubic (c-BN) and hexagonal (h-BN) polytypes as a prototypical system for the renormalization of optical properties in semiconductors by lattice vibrations. While band-gap renormalization due to electron-phonon coupling is a well-explored concept in semiconductor physics, this topic has gained renewed attention in the context of pump-probe spectroscopies where high fluences may lead to local lattice excitation. With this motivation, we performed first-principles calculations of c-BN and h-BN supercells using the DFT+GW method, treating lattice excitation via explicit atomic displacements. Finally, the frequency-dependent dielectric function and the optical absorbance are obtained including many-particle effects on the level of the Bethe-Salpeter equation. The results show that the atomic displacements in the 2x2x2 supercells used in this study have little effect in c-BN but lead to a considerable narrowing of the optical gap in h-BN. In h-BN, the band splitting due to 'frozen' phonons gets even amplified on the GW level of theory. The binding energy of approximately 0.5eV of the exciton derived from the band edges, however, is found to be only weakly affected by the atomic displacements.

Financial support from CRC 1242 is gratefully acknowledged.

HL 35.9 Wed 18:45 POT/0251

Half-saddle excitons in monolayer SnS2: a first-principles study — •Vinicius Alves Bastos[1], Fulvio Paleari[2], Eleonora Luppi[3], Marco Gibertini[1,2], and Alice Ruini[1,2] — [1]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Modena (Italy) — [2]CNR-Nano, Modena (Italy) — [3]Laboratoire de Chimie Théorique, Sorbonne Université and CNRS, Paris (France)

Monolayer SnS2 has been demonstrated as a visible-light absorber with promising characteristics for applications in fuel cells and thin film photovoltaics [1]. Motivated by that, we have performed a first-principles study of bound excitons in this system within the GW-BSE formalism [2]. We have gone beyond previous works by analysing the exciton symmetries, electron-hole contributions, and transition dipoles. We find a richer structure of bound excitons than previously reported, e.g., deeply bound dark excitons with binding energies of about 0.9 eV and a very strong bright exciton at 2.9 eV, in good correspondence with the experimental absorption peak. Also, the bound excitons are localized around the direct band gap at the M point, which exhibits a saddle point at the top valence band and a minimum at the bottom conduction band. Consequently, we show that linearly polarized light can be used to completely select two of the three inequivalent M saddles, as previously demonstrated in graphene [3]. PNRR MUR project ECS_00000033_ECOSISTER

[1] Y. Sun et al., Angew. Chem. Int. Ed. 51, 8727 (2012). [2] D. Sangalli et al., J. Phys. Condens. Matter. 31, 325902 (2019). [3] S. Sharma et al., arXiv preprint, arXiv:2503.21376 (2025).

HL 36: 2D Materials VI – Optoelectronic properties

Time: Wednesday 17:30–18:30 Location: POT/0081

HL 36.1 Wed 17:30 POT/0081

Surface acoustic wave-controlled photocurrent in few-layer WSe2 — •Benjamin Mayer, Felix Ehring, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

Surface acoustic waves (SAWs) offer a versatile platform for nanoscience applications [1]. Their ability to integrate GHz-frequency control and sensing schemes at micron-scale wavelengths on a chip opens cross-disciplinary applications and enables the SAW electric field to drive acousto-electric currents in low-dimensional materials, including semiconducting transition metal dichalcogenides (TMDCs) [2]. Here, we study the AEC and the underlying charge-carrier dynamics in mechanically exfoliated 2D tungsten diselenide (WSe2) placed on two gold electrodes integrated into hybrid lithium-niobate-based SAW devices (150-250 MHz). Our multifunctional acousto-optoelectric setup combines current-voltage characterization, SAW-direction dependent AEC measurements and spectrally resolved scanning photocurrent (PC) spectroscopy. This allows detailed investigation of how electrical contacts affect the performance of our archetypical acoustophotoelectric device. Thus, we establish a qualitative model of the tunneling barrier and band bending induced by Schottky barriers at the Au-TMDC interface [3]. Further, tuning the optical excitation wavelength provides spectral access to energy-dependent photocurrent contributions and reveals how they are modulated by the SAW.

[1] Krenner, J. Phys. D: Appl. Phys. (2025, subm.) [2] Nat. Comm. 6 (1): 8593 (2015) [3] ACS Appl. Electr. Mat. 7 (21): 9717 (2025)

HL 36.2 Wed 17:45 POT/0081

Shift current tuned via twisting angle in moiré system — •Michele Bagaglini[1,2], Cesare Tresca[2], and Gianni Profeta[1,2] — [1]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy — [2]CNR-SPIN c/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy

In recent years the interest in the two-dimensional bulk photovoltaic effect (BPVE) has been increasing in non-centrosymmetric materials. Research on 2D solar cells and optoelectronic device is focusing on these materials due to their highly efficient response. The shift current (SC) is one of the most important effect to the BPVE. The SC is second-order non-linear response that arises from the different real-space centres position of charge, a 'shift', between the valence and conduction bands. In the literature, several studies already exist on the SC in monolayer and untwisted bilayer transition-metal dichalcogenide (TMD) systems, where promising peaks have been reported from DFT calculations. In this study we focus on the evolution of the SC with the twisting angle in moiré twisted two-dimensional materials, specifically in multilayer MoS2 systems. In our case, given the large size of the systems for small twist angles, we employ a tight-binding (TB) approach with Slater-Koster (SK) parameterization to compute the SC. We show that a multiband approach improves the accuracy and allows one to reproduce the dispersions obtained from first-principles calculations.

HL 36.3 Wed 18:00 POT/0081

Theoretical investigation of the flexo-photovoltaic effect — •Juan Jose Esteve-Paredes[1], Maria N. Gastiasoro[2], and Julen Ibanez-Aspiroz[1] — [1]Materials Physics Center, University of the Basque Country, Donostia-San Sebastian, Spain — [2]Donostia International Physics Center, Donostia-San Sebastian, Spain

The bulk photovoltaic effect (BPVE) refers to the generation of a direct current in a bulk crystal under illumination. This phenomenon arises in non-centrosymmetric materials and is described by a finite electronic

second-order conductivity. In recent years, experimental works have reported the realization of the BPVE in centrosymmetric media, where this effect is conventionally forbidden, by generating large strain gradients through application of local pressure with nanoscale tips [1,2]. This new effect, named the flexo-photovoltaic effect, has attracted interest regarding its microscopic origin. In this talk, we theoretically investigate this effect and demonstrate that a flexo-photovoltaic effect can indeed be predicted by considering local lattice deformations in several-layer centrosymmetric crystals, giving rise to the appearance of a finite BPVE conductivity. We employ a Slater-Koster approach to model the electronic band structure and wavefunctions within a supercell geometry and compute the associated linear and second-order optical responses. We discuss the tunability and scaling of this effect in relation to the magnitude and spatial extent of the mechanical deformation, and discuss how our theoretical predictions compare with existing experimental observations. [1] Yang et al., Science 360, 904 (2018) [2] Wang et al., Phys. Rev. Lett. 132, 086902 (2024)

HL 36.4 Wed 18:15 POT/0081

All-in-one Optoelectronic Synaptic Device with Van der Waals materials-based floating gate — •Thi Phuong Anh Bach and Sangeun Cho — Division of System Semiconductor, Dongguk University, Seoul, South Korea

Optoelectronic synaptic devices that integrate nonvolatile memory with light matter interactions offer high processing efficiency and low energy consumption for neuromorphic computing. Two-dimensional materials and their van der Waals heterostructures provide strong electronic and optical properties, while floating-gate structures emulate synaptic plasticity and enable a path toward brain-inspired, beyond-von-Neumann computation. Herein, we demonstrate a multifunctional optoelectronic synapse device based on rhenium disulfide (ReS2)/hexagonal boron nitride (hBN)/indium selenide (InSe) vdW FG structure. The device exhibits a high On/Off current ratio (>10^6), large memory window, multi-level storage behavior and excellent data retention (~10000 s) under various electrical and optical stimuli. By leveraging the thickness tunalble bandgap of InSe FG and the dynamic tunneling process of photogenerated carriers across the vdWhs interface, the device capable to work under a wide range from visible to near-infrared laser with excellent synaptic plasticity. The device replicates classical conditioning (Pavlov's dog experiment) and advanced signal-discrimination learning, and also supports reconfigurable inverter logic via electrical and optical inputs, along with neuromorphic image recognition, demonstrate its multifunctionality.

HL 37: Nitrides II – Designed properties and LED

Time: Thursday 9:30–11:00 Location: POT/0006

HL 37.1 Thu 9:30 POT/0006

Designing Visible-Spectrum Nitride Alloys from First Principles — •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

Precise band-gap engineering across the full visible spectrum is essential for emerging applications such as integrated RGB LEDs. This tunability can be achieved through alloying narrow-band-gap materials like InN or ScN with wide-band-gap semiconductors such as GaN or AlN. Among these systems, random alloys including (In,Ga)N and (Al,Sc)N require advanced theoretical treatments–such as the coherent potential approximation (CPA) and special quasi-random structures (SQS)–to capture their configurational disorder accurately.

In this work, we combine first-principles density functional theory with efficient electronic-structure methods such as LDA-1/2 and the mBJ functional to provide a comprehensive dataset for both random and ordered alloy phases. We report key structural properties including lattice parameters and bond lengths as well as elastic constants, phonon modes, thermodynamic stability, and electronic characteristics such as band gaps and Bloch spectral functions. These results offer a robust theoretical foundation for experimental detection of ordering phenomena and for the rational design of nitride alloys with tailored optical and electronic properties.

HL 37.2 Thu 9:45 POT/0006

Detailed nano-characterization of structural and optical properties of a red-emitting InGaN LED — •N. Dreyer[1], F. Bertram[1], G. Schmidt[1], J. Christen[1], Z. Chen[2], and X. Wang[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Peking University, Beijing, China

A fully processed and operating red InGaN LED was grown by MOVPE on a GaN/sapphire template. The active region, which consists of three identical stacks, is surrounded by n- and p-GaN with an EBL. Each stack contains three quantum wells with different indium concentrations: two with a low indium concentration for strain relaxation, and one subsequently grown red-emitting quantum well (RQW). The structure was characterized using scanning transmission electron microscopy (STEM) and the orientation of the Burgers vector (edge- or screw type dislocation) was determined. Cross-sectional cathodoluminescence performed directly in STEM shows broad band-to-band recombination in the n-GaN at $T = 17$ K which is caused by band gap renormalization and conduction band filling. Line shape analysis of this emission band yields a charge carrier density of 6×10^{18} cm^{-3}. The vertical evolution of the RQW emission exhibits a shift of 123 meV within the active region. Furthermore, the lateral homogeneity of the RQW emission will be examined. A blue-shift of the RQW emission of up to 365 meV was found around defects. The vertical and lateral trapping processes of excess carriers will be discussed in detail. The capture length of the bottom RQW was found to be 78 nm using highly spatially resolved vertical linescans across the active region.

HL 37.3 Thu 10:00 POT/0006

Determination of optical losses in AlGaN-based multimode waveguides — •Verena Kowallik[1], Martin Guttmann[2], Leonardo Wildenburg[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute for Physics & Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs), such as biochemical sensing, atomic clocks, and UV Raman spectroscopy, require materials with a large bandgap energy to facilitate low optical losses. One possible candidate are AlGaN alloys which are already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN materials, especially the absorption losses have not yet been studied in detail in the UVC spectral range. In this work, the absorption losses in 200 μm wide n-$Al_{0.76}Ga_{0.24}N$ waveguides were investigated using monolithically integrated UV-LEDs emitting at 262 nm and detectors. By Monte Carlo ray-tracing simulations, we identified different contributions of the optical losses, namely, the propagation losses and scattering losses. Here, we implemented the waveguide surface roughness determined from atomic force microscopy images. Also, we investigated the portion of rays reaching the detector without beeing guided in the waveguide, e.g. scattered at the substrate's backside or the AlN/sapphire interface.

HL 37.4 Thu 10:15 POT/0006

Influence of the AlGaN multi-quantum well design on the efficiency of 233 nm far-UVC LEDs grown by MOVPE — •Rebekah Seonggyeong Kim[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Physics and Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Light emitting diodes (LEDs) emitting in the far ultraviolet-C (far-UVC) spectral range are promising for applications like skin safe disinfection and gas sensing. The composition and thickness of the AlGaN-multi quantum wells and barriers are crucial for the efficiency of the LEDs. In this work we investigate the impact of the last quantum well barrier's (LB) thickness (0 nm to 10 nm) and aluminum mole fraction (76% - 86%) onto the electrooptical performance of the LEDs. The LEDs with an aluminum mole fraction of 80 % and a thickness of 5 nm exhibit the highest external quantum efficiency (EQE) of 0.32 % at 16 mA (on-wafer).

HL 37.5 Thu 10:30 POT/0006

In-rich InGaN quantum well growth for green InGaN LED — •Christoph Berger, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-University, Magdeburg, Germany

Achieving high-efficiency green InGaN LEDs remains challenging due to material issues like phase instability, metallic inclusions and interface roughening. We present an optimized MOVPE growth approach that significantly improves the optical and morphological quality of green LEDs. After each QW, a growth interruption combined with a controlled temperature ramp is introduced before starting the GaN barrier growth. This sequence allows to get rid of excess indium that accumulates on the surface during QW growth, leading to smoother interfaces, a removal of indium-rich defects visible in Nomarski microscopy and consequently, a substantial suppression of a grayish appearance of the wafer. We further combine this process with hybrid MQW designs, where blue QWs are grown below a green top QW, leading to an improvement of the efficiency of the LED. The impact of different growth sequences and layer designs on the optical and structural characteristics of green LEDs will be discussed.

HL 37.6 Thu 10:45 POT/0006

Nano-characterization of polarization-doped deep UV LED structures using highly spatially resolved cathodoluminescence spectroscopy — •E. Bäker[1], F. Bertram[1], G. Schmidt[1], N. Dreyer[1], J. Christen[1], T. Kolbe[2], S. Hagedorn[2], H.K. Cho[2], J. Rass[2], S. Einfeldt[2], and M. Weyers[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Ferdinand-Braun-Institut (FBH), Germany

AlGaN-based deep UV LEDs emitting below 250 nm are of great interest for many applications. Especially in the far-UVC, efficient p-doping poses major challenges, which can be effectively overcome by the concept of polarization doping. This study compares far-UVC LEDs with different AlGaN composition gradients used for polarization doping. The LEDs were grown by MOVPE on optimized AlN/sapphire templates. While the n-side of the diode uses conventional Si-doping, the p-side utilizes an AlGaN-layer with constant [Ga]-gradient. Diodes with different [Ga]-gradients but identical thicknesses are analyzed, with the Ga mole fraction increasing linearly from 0.02 to 0.45 and from 0.02 to 0.81, respectively. Using low temperature cathodoluminescence spectroscopy directly performed in a scanning transmission electron microscope, a nano-scale correlation of the optical properties with the real structure is obtained. Cross-sectional CL line scans show the different emission of the gradient layer. While the sample with the shallow gradient shows continuous emission spectral red-shift from 240 nm to 260 nm, the sample with the steep gradient shows an abrupt jump from 273 nm to 312 nm, indicating lattice relaxation.

HL 38: Materials and Devices for Quantum Technology II

Time: Thursday 9:30–12:45 Location: POT/0051

HL 38.1 Thu 9:30 POT/0051

Shadow masks for all-in-situ fabrication of InAs nanowire Josephson junctions — •Christian Schäfer, Lennart Grosch, Yurii Kutovyi, Nils von den Driesch, Thomas Schäpers, and Alexander Pawlis — PGI 9 / PGI 10 / JARA-FIT, Forschungszentrum Jülich, 52428 Jülich, Germany

Josephson junctions based on semiconductor/superconductor hybrid structures offer unique features for quantum circuits, such as gate-controllable supercurrent and quantized Andreev bound states. Clean interfaces between nanowire and superconductor are essential to leverage both effects, driving the development of in-situ contact fabrication. Shadow wall epitaxy offers both, a scalable and all-in-situ solution for nanowire growth and contact formation. Micrometer-high pre-fabricated walls shadow the molecular beams of In and As depending on their relative orientation. Since As on its own has a low sticking coefficient and In forms isolated droplets, partially shadowed regions are insulating and do not form InAs crystals. Despite the significant lattice mismatch between InAs and the GaAs substrate, we observe growth of lateral 1D-nanowires between walls spaced less than one micrometer. The same mask can additionally be used to perform selective deposition of any superconductor. We explore different mask designs to optimize electrical device isolation, nanowire growth, and junction geometry. Since no transfer or post-processing after growth is necessary, associated defects and degradation are avoided. Shadow wall epitaxy enables scalable in-situ fabrication of InAs nanowire junctions.

HL 38.2 Thu 9:45 POT/0051

Semiconductor−superconductor membranes for nanoelectronic devices — •Thies Jansen[1], Christian Reichl[2], and Thomas Sand Jespersen[1,3] — [1]Technical University of Denmark, Anker Engelunds Vej 101 2800 Kongens Lynby — [2]ETH Zürich Laboratorium für Festkörperphysik — [3]Center for Quantum Devices Niels Bohr Institute, University of Copenhagen

Semiconductor-superconductor hybrid materials have become the workhorse platform for quantum devices, owing to their clean and highly transparent semiconductor-superconductor interfaces. Indium arsenide−aluminum (InAs-Al) nanowires and quantum wells are currently the dominant material systems, each offering distinct advantages: nanowires allow transfer to arbitrary substrates, while quantum wells provide two-dimensional design flexibility. Here, we introduce a new platform that combines the strengths of both systems: a semiconductor-superconductor membrane. We present the fabrication of these membranes and their initial electrical characterization through low-temperature transport measurements. The membranes are gate-tunable, and their material properties closely resemble those of both InAs nanowires and InAs quantum wells.

HL 38.3 Thu 10:00 POT/0051

Secondary electron detector for deterministic single ion implantation — •Priyal Dadhich, Nico Klingner, and Gregor Hlawacek — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf(HZDR), Dresden, Germany

Fault tolerant quantum computers based on donor-ion solid-state qubits require highly localized placement of single donors. To achieve this, we are developing a new setup for deterministic single-ion implantation in a FIB. To detect each implanted ion, we aim to use the secondary electrons (SEs) emitted during ion impact. A windowless silicon drift detector (SDD), biased up to +10 kV, accelerates and collects these SEs. The resulting electron-hole pairs allow us to quantify the number of emitted electrons via pile-up analysis. A critical challenge for this detection approach is the intrinsic SE emission probability. As governed by Poisson statistics, the average SE yield strongly affects detection confidence. Current work examines material-dependent absolute SE yields and practical methods to enhance SE emission while maintaining efficient extraction. Given the low SE yield per impact, optimizing the extraction geometry is crucial. A C++ simulation code using the ion-optics library IBSIMU [1] has been developed for this customised problem, to maximize SE collection and study backscattering, including possible methods to recollect backscattered electrons. References: [1] T Kalvas et. al. Rev. of Sci. Inst., 81(2), 2010.

HL 38.4 Thu 10:15 POT/0051

Spin-orbit-enabled realization of arbitrary two-qubit gates on moving spins — •David Fernández-Fernández[1], Yuta Matsumoto[2], Lieven M.K. Vandersypen[2], Gloria Platero[1], and Stefano Bosco[2] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — [2]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

Shuttling spin qubits across semiconductor quantum dot arrays is emerging as a key primitive for scalable quantum information processing, enabling on-chip inter-node quantum communication and modular architectures. By analyzing the shuttling of two spin qubits towards each other using a conveyor-mode protocol, we show that controlling only two experimentally accessible parameters, the shuttling velocity and the waiting time at minimum interdot separation, is sufficient to synthesize a broad class of entangling gates. Moderate SOI provides direct access to both CPHASE(θ) and SWAP$^\alpha$ families, as well as native fermionic-simulation gates, all with fidelities above 99.99% neglecting decoherence. We further quantify gate accessibility through a Weyl-chamber analysis and demonstrate that strong SOI or engineered helical magnetic fields can unlock nearly complete ($\sim$ 99.98%) coverage of all locally inequivalent 2Q operations, including quantum gates such as the Berkeley gate. This work provides a realistic and

scalable route toward single-step 2Q gates on mobile spin qubits, with immediate implications for distributed quantum computing, quantum simulation, and shuttling-assisted error-correcting architectures.

HL 38.5 Thu 10:30 POT/0051

Topological Superconductivity in the Presence of Contact Potentials — •Leonard Kaufhold — Institute for Theoretical Physics, Cologne, Germany

The research on Majorana bound states (MBS) has brought forth a multitude of proposed platforms and devices that are, in principle, capable of realizing such states as topological edge modes. These devices usually rely on the superconducting proximity effect induced in semiconductors with strong spin-orbit coupling or, more recently, in topological insulators. The material interface however induces another effect that can be as much as one order of magnitude larger than the electronic band gap at the surface. Due to the mismatch of work functions between the materials, a dipole layer forms at the interface, effectively creating a contact potential that modifies the electronic band structure far beyond the minimal models typically used to describe the formation of MBS. In this presentation, we will focus on different nanowire-based architectures consisting of a topological insulator in contact with an s-wave superconductor, and discuss on a theoretical level the effect of contact potentials on the formation and stability of MBS. We further outline under which parameter conditions these interface-induced effects become experimentally relevant.

HL 38.6 Thu 10:45 POT/0051

Hexagonal Germanium Nanowires as a Spin Qubit Platform — •Anirban Das[1], Baksa Kolok[1,2], Daniel Varjas[1,3], and Andras Palyi[1,2] — [1]Department of Theoretical Physics, BME, Budapest, Hungary — [2]HUN-REN-BME-BCE QTRG, BME, Budapest, Hungary — [3]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany

Hexagonal germanium (2H-Ge) offers strong spin-orbit interaction and optical activity, making it an appealing platform for semiconductor spin qubits. Recent progress in growing hexagonal Si_xGe_{1-x} nanowires enables controlled geometries suitable for quantum devices. In contrast to cubic Si or Ge, 2H-Ge supports direct band-gap transitions, opening a pathway towards a novel spin-photon interface.

We study the electronic and spin properties of 2H-Ge nanowires using a multiband k·p Hamiltonian describing low-energy states near the Γ point. By discretizing the model with open boundaries, we construct nanowires oriented perpendicular to the c-axis and compute their band structure. We analyze confinement-induced gap variations and the influence of transverse electric fields, from which we extract Rashba coefficients. Magnetic fields are included via a Peierls substitution to investigate anisotropic spin responses. The resulting effective g-tensor shows strong directional dependence, revealing regimes favorable for qubit operation in hexagonal Ge nanowires.

This research is supported by the European Union within the Horizon Europe research and innovation programme via the ONCHIPS project under grant agreement No 101080022.

15 min. break

HL 38.7 Thu 11:15 POT/0051

Low-Loss LNOI PIC Components for Quantum Interference Applications — •Mohammad Malik[1,2,3], Simon Palitza[1,2,3], and Carsten Schuck[1,2,3] — [1]Department for Quantum Technology, University of Münster — [2]Center for NanoTechnology - CeNTech, Münster — [3]Center for Soft Nanoscience - SoN, Münster

Lithium niobate on insulator (LNOI) exhibits significant potential as a platform for integrated photonics owing to its strong electro-optic response, broad transparency window, and intrinsic nonlinear properties. For on-chip quantum key distribution (QKD) and related quantum photonic applications, the precise fabrication of photonic integrated circuit (PIC) components with minimal loss and high fidelity remains a key challenge. Here, we demonstrate directional couplers (DCs) and multimode interferometers (MMIs) that achieve a 50/50 splitting ratio with insertion losses below 1.5 dB at a wavelength of 1550 nm. These results are obtained using in-house fabrication techniques, including electron-beam lithography and inductively coupled plasma reactive ion etching, enabling accurate and reproducible realization of crucial PIC components. Building on these results, we will discuss progress towards integrating superconducting nanowire single-photon detectors (SNSPDs) on the LNOI platform for realizing on-chip Hong-Ou-Mandel interference as required for integrated quantum technology applications, including measurement device independent QKD.

HL 38.8 Thu 11:30 POT/0051

Scalable and individual control of Si qubits via magnetic skyrmions — •Leander Reascos[1], Raluca Boltje[1], Kai Litzius[1], Felix Büttner[1,2], and Mónica Benito[1] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

Scalable, precise control of spin qubits is essential for large-scale quantum processors with millions of qubits. Electron-spin qubits in semiconductor quantum dots are promising due to their small size, high fidelities, long coherence times, and CMOS compatibility. However, current electric-dipole spin resonance (EDSR) schemes rely on static micromagnets, which suffer from fabrication-induced inhomogeneities and limited tunability. We propose using gate-tunable nanoscale magnetic skyrmions as on-chip magnetic field sources to replace micromagnets. By controlling skyrmion geometry, the local magnetic field at a quantum dot can be tuned post-fabrication to adjust both the qubit frequency and the EDSR driving gradient. Using micromagnetic simulations and analytical modeling, we show how skyrmion geometry maps directly onto the qubit's Zeeman splitting and Rabi frequency. These results highlight skyrmion-based control as a promising route towards scalable, frequency-selective spin-qubit architectures with enhanced tunability.

HL 38.9 Thu 11:45 POT/0051

Strain modulation in Germanium: an overview for quantum applications — •Meera None[1], Ignatii Zaitsev[1], Davide Spirito[2], Patricio Farrell[3], Christian Merdon[3], Yiannis Hadjimichale[3], Daniel Fritsch[4], Marvin Hartwig Zoellner[1], and Costanza Lucia Manganelli[1] — [1]IHP-Frankfurt (Oder)-Germany — [2]BC-Materials-Leioa, Spain — [3]WIAS-Berlin — [4]Zuse-Berlin

Germanium (Ge) is a promising platform for hole-based quantum devices due to its high hole mobility, strong spin-orbit coupling, and compatibility with CMOS technology. We investigate strain engineering in an ideal structure with two silicon nitride (SiN) stressors on a Ge substrate, using FEM to study how stress level, stressor height, and design influence mechanical deformation. The resulting strain tensors, including often neglected shear components, are inserted into a fully coupled 6x6 Bir-Pikus Hamiltonian to compute heavy hole (HH) and light hole (LH) band shifts under uniaxial and biaxial stress. Our results show tunable HH-LH splitting from 36 to 165 meV for SiN stressors between 1 and 4 GPa, demonstrating that SiN stressors offer a practical, scalable route to engineer Ge band structure for quantum wells and hole spin qubits.

HL 38.10 Thu 12:00 POT/0051

Optical probing of strain fields in isotopically pure Si-28 using donor-bound excitons — •Nico Eggeling[1], Phillip Külper[1], N.V. Abrosimov[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

The successful demonstration of all optical qubits in isotopically pure Si-28 utilises the donor-bound exciton transition of phosphorus dopants [1]. As a current obstacle for large-scale implementation, the challenge remains to harness inhomogeneities resulting from simple imperfections in the crystal lattice, over dopant-dependent lattice deformations, to even the hydrostatic pressure due to the sample's own weight or adjacent interfaces. We present results from spatially resolved measurements of the donor-bound exciton, revealing a distinct strain distribution in a bulk Si-28 sample at cryogenic temperatures. These are explained in the context of the Pikus-Bir formalism for silicon [2], leading to strain estimates that are well matched to the known extrinsic factors.

[1] E.Sauter, PhD Thesis (2022)
[2] Loippo et al., Phys. Rev. Mater. 016202 (2023)

HL 38.11 Thu 12:15 POT/0051

Development of heavy noble gas field ion sources using an iridium coated single crystalline tungsten emitter — •Amina Zid[1,2], Gregor Hlawacek[1], Nico Klingner[1], Arnaud Houel[2], and Anne Delobbe[2] — [1]Institute for Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]ORSAY PHYSICS, 95, 3ème Avenue - ZA Saint-Charles, 13710 Fuveau, France

Gas Field Ion Sources (GFIS) provide high brightness, high current density and excellent spatial resolution[1]. Conventional GFIS use light noble gases: helium enables 0.5 nm imaging resolution, while neon allows high-resolution milling beyond Liquid Metal Ion Source (LMIS) capabilities. However, low maximum current limits material removal rates, and the light ions cause deep implantation and bubble formation, reducing efficiency for large-volume or high-aspect-ratio milling. To overcome these limits, we investigate GFIS operation in a Focused Ion Beam (FIB) using heavier noble gases.

Additionally an iridium-coated tungsten tip is investigated. Iridium forms the strongest bond with tungsten[2], enabling higher electric fields and thus higher stable beam currents. Our emitter operates from a single emission point rather than the typical trimer used in Helium Ion Microscopy. This work presents the first FIB performance evaluation of this emitter with argon and xenon, including comparison to helium and neon-based GFIS.

[1] Höflich, K. et al., Applied Physics Reviews 2023; G. Hlawacek & A. Gölzhäuser (Eds.), Helium Ion Microscopy, Springer, 2016.

[2] Oshima, C. et al., Surface Science and Nanotechnology 2018.

HL 38.12 Thu 12:30 POT/0051

Finding the kinked propagation of the I3 defect in hexagonal silicon using a machine-learned potential — •Jolijn Dellevoet — Eindhoven University of Technology, Eindhoven, The Netherlands

Hexagonal silicon-germanium (hex-SiGe) alloys have recently emerged as promising direct-bandgap semiconductors suitable for on-chip optical communication, offering a path to reduce heat production in microchips. Currently, the hex-SiGe crystal is grown in core-shell nanowire structures, but their crystal quality is hindered by the formation of I3 defects. During growth, these defects nucleate and can propagate into otherwise pristine crystal. This propagation has been observed experimentally but not reproduced in atomistic simulations, leaving the underlying mechanism unclear. This presentation reveals, at atomic resolution, a kinking mechanism that enables the I3 defect boundary to propagate within hex-Si. This mechanism and its corresponding energy landscape are obtained by using the nudged elastic band (NEB) method in combination with the machine-learned PACE potential. Although the calculations are currently limited to Si systems, future studies could focus on extending the calculations to SiGe systems. The temperature and boundary length dependence of the transition rate can ultimately be used to optimize growth conditions of the hex-SiGe core-shell nanowires.

HL 39: 2D semiconductors VII – CrSBr and related heterostructures

Time: Thursday 9:30–12:30 Location: POT/0081

HL 39.1 Thu 9:30 POT/0081

Ab initio investigation of electronic, magnetic, optical properties and proximity effect in MoS_2/CrSBr van der Waals heterostructures — •Athanasios Koliogiorgos and Karel Carva — Charles University, Prague, Czech Republic

CrSBr-MoS_2 heterostructures combine the properties of the antiferromagnetic semiconductor CrSBr and the TMD semiconductor MoS_2, yielding a promising platform for spintronic and valleytronic applications. In connection with experimental work, using density functional theory with GGA+U and hybrid HSE06 functionals, we explore the structural, electronic, magnetic and optical properties of MoS_2/CrSBr systems, where CrSBr is 1-4 layers thick and MoS_2 a monolayer. We observe induced magnetization in the MoS_2 layer via proximity effect, strongly dependent on the interlayer distance. Other proximity effects include charge transfer, bandgap renormalization and spin splitting in the band structure, while the density of states reveals a weakly hybridized system, retaining the characteristics of the separate parts. Work function and band alignment show that the material behaves as a Type-II heterostructure. The calculation of the absorption coefficient reveals distinct peaks corresponding to the CrSBr and MoS_2 layers, in agreement with the experimental photoluminescence spectrum.

HL 39.2 Thu 9:45 POT/0081

Proximity-Induced Raman Signatures in a $NbSe_2$-CrSBr Superconductor-Magnet Heterostructure — •Elena Vinnemeier[1], Jan-Hendrik Larusch[1], Kai Rossnagel[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

Interfacing superconducting $NbSe_2$ with the antiferromagnetic semiconductor CrSBr provides a van der Waals platform to study proximity effects in quantum devices. The superconductivity-magnetism interplay enables Josephson junctions and superconducting quantum interference devices with field-tunable critical current and spin filtering. We study proximity effects of the spin ordered CrSBr on the specific collective modes in $NbSe_2$ in the superconducting phase at 4K and the charge-density wave phase at 15K. A magnetic field tunes CrSBr from antiferromagnetic to ferromagnetic order. The Raman response of the heterointerface, relative to bare $NbSe_2$, reveals proximity effects from the ferromagnetic CrSBr layer at the interface. Modifications of the $NbSe_2$ collective excitation spectrum demonstrate strong interaction between the proximitized magnetic order in CrSBr and correlated phases in $NbSe_2$. This project was supported by the EIC pathfinder grant 101130224 "JOSEPHINE".

HL 39.3 Thu 10:00 POT/0081

Exciton dominated anisotropic dielectric tensor in CrSBr — •Jan-Hendrik Larusch[1], Pierre-Maurice Piel[1], Aleksandra Łopion[1], Thomas Kliewer[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

CrSBr is an air-stable magnetic vdW semiconductor with a direct bandgap; its anisotropic spin, lattice, and charge, drive anisotropic light-matter interaction $\varepsilon(\omega)$. We directly determine the full dielectric tensor of exfoliated CrSBr by spectroscopic imaging ellipsometry (SIE). In the paramagnetic phase, SIE verifies $\varepsilon_{xx} \times \varepsilon_{yy} \times \varepsilon_{zz}$. Room-temperature comparison of Mueller-matrix and generalized ellipsometry guides cryogenic SIE, enabling us to track changes across the Curie and Néel temperatures as the system evolves from paramagnetic over intralayer ferromagnetism to A-type antiferromagnetism. In the AFM phase, polarization-resolved magneto-reflectance with fields along c (hard), b (easy), and a (intermediate) axis yields critical fields of roughly 2.2, 1.05, and 0.3 T for transition to FM order sensed by distinct optical fingerprints. Together, these measurements quantify the anisotropic light-matter interaction and its dependence on magnetic order, linking exciton-dominated emission/absorption to the full dielectric tensor [1]. [1] J. Klein et al. ACS Nano 17, 5316-5328 (2023).

HL 39.4 Thu 10:15 POT/0081

Optical Probing of Interfacial Magnetic Properties of the CrSBr-$MnPS_3$ hetero-interface — •Thomas Kliewer[1], Aleksandra Łopion[1], Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]University of Münster, Germany — [2]University of Chemistry and Technology Prague, Czech Republic

CrSBr and $MnPS_3$ are both 2D antiferromagnetic semiconductors with different magnetic and optical properties. $MnPS_3$ has out-of-plane spin alignment while CrSBr's spins are aligned in-plane [1,2]. Interfacing these two materials is expected to result in complex interfacial spin-alignment, presumably with the stabilization of a non-collinear magnetic phase at the interface. CrSBr exhibits strong excitonic features coupled to the magnetic order [3]. This is used as a probe for the magnetic situation of the $MnPS_3$-CrSBr interface. The structures are characterized by polarization-resolved Raman spectroscopy measurements and the interfacial magnetic properties are probed by low-temperature magneto-photoluminescence and reflectance spectroscopies. We observed a peculiar influence of $MnPS_3$ on the optical response of CrSBr. A proximity-induced modification of the magnetic properties of CrSBr interfaced with $MnPS_3$ seems to induce long-range order, since the impact is observable on the CrSBr flake more than 10 μm away from the interfaced region. Our observations might be connected to the stabilization of an intermediate ordered magnetic state in CrSBr. [1] Wilson, et al. Nat. Mat. 20.12 (2021), [2] Kobets, et al. Low Temp. Phys. 35.12 (2009), [3] Heißenbüttel, et al. Phys. Rev. B 111.7 (2025)

HL 39.5 Thu 10:30 POT/0081

Coupling Between Vibrational, Electronic, and Magnetic States in CrSBr — •Daria Markina[1], Priyanka Mondal[1], Lukas Krelle[1], Sai Shradha[1], Mikhail M. Glazov[2], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]St. Petersburg, Russia — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

The van der Waals antiferromagnet CrSBr displays interplay between vibrational, electronic, and magnetic states, producing distinctive quasiparticle interactions. Using temperature-dependent polarization-resolved Raman spectroscopy with optical absorption and photoluminescence excitation (PLE), we examine these effects across the magnetic phase transition. Under 1.96 eV excitation, the A_g^1, A_g^2, and A_g^3 Raman modes exhibit pronounced polarization and intensity changes near the Néel temperature, accompanied by modifications in excitonic oscillator strength and resonant PLE features. The distinct temperature evolution of Raman tensor elements indicates that individual phonons couple to specific excitonic and electronic states. The suppression of excitonic transitions above the Néel temperature links these effects to spin alignment, suggesting an indirect spin−phonon interaction mediated by exciton−phonon coupling. These findings establish CrSBr as a promising platform for studying quasiparticles in two-dimensional magnets and for potential quantum technologies.

HL 39.6 Thu 10:45 POT/0081

Evidence for a novel spin-density excitation in 2D magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Aleksandra Łopion[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 magnet CrSBr is an air-stable semiconductor with ferromagnetic layers, antiferromagnetic interlayer coupling, and a highly anisotropic bandstructure, resulting in quasi-one-dimensional excitonic states [1]. We probe the impact of magnetic order on excitons and collective modes using low temperature (4K) magneto photoluminescence and resonant Raman spectroscopy with special emphasize on the magnetic anisotropy and magnetic phase transitions. The excitonic signatures in photoluminesence show clear differences between antiferromagnetic and ferromagnetic regimes and reveal pronounced magnetic anisotropy. In resonant Raman, the first order Ag phonons remain essentially field independent, whereas additional modes appear only under excitonic resonance. We resolve a sharp mode near 248 cm-1 emerging in resonance with the A-exciton (˜1.36eV) and a broad mode at 362 cm-1 occurring in A and higher-lying excitonic regimes. The mode's excitation energy and field dependence indicate selective access to different collective possibly spin-density excitations in CrSBr.
[1] J. Klein et al., ACS Nano 17, 5316-5328 (2023).

15 min. break

HL 39.7 Thu 11:15 POT/0081

Tracking Magnetic Phase Evolution in CrSBr via Excitonic Emission and Absorption — •Lukas Krelle[1], Ryan Tan[1], Daria Markina[1], Priyanka Mondal[1], Kseniia Mosina[2], Kevin Hagmann[1], Regine von Klitzing[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

CrSBr is an air-stable magnetic van der Waals semiconductor, in which the interaction of excitons with the magnetic order enables the optical identification of different magnetic phases. Here, we study multi-layer samples of CrSBr inside a three-axis vector magnet and correlate magnetic order and optical transitions. We identify layer by layer switching of the magnetization through drastic changes of the optical absorption energy and strength as a function of the applied magnetic field. We find that ferromagnetic and antiferromagnetic order between layers can coexist in the same domain [1]. The photoluminescence evolution depends on the magnetic order and can differ for each emission. The intensity of energetically lower lying transitions reduces monotonously with increasing field strength whereas energetically higher lying transitions around the bright exciton increase in intensity close to the saturation field. Using this contrasting behavior we can therefore correlate transitions with each other.
[1]: L. Krelle et al, ACS Nano 2025, 19, 33156

HL 39.8 Thu 11:30 POT/0081

Magnetically controllable exciton-polariton condensation in CrSBr microwires — •Christian Weidgans[1], Heng Zhang[1], Niloufar Nilforoushan[1,4], Julian Hirschmann[2], Marlene Liebich[1], Tobias Inzenhofer[1], Imke Gronwald[1], Josef Riepl[1], Kseniia Mosina[3], Zdeněk Sofer[3], Fabian Mooshammer[1], Florian Dirnberger[2], and Rupert Huber[1] — [1]University of Regensburg, Germany — [2]Technical University of Munich, Germany — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Université Paris Cité, France

Coupling the macroscopic wave functions of quasiparticle condensates to other degrees of freedom, such as the electron spin, could offer valuable control knobs for future quantum applications. In particular, man-made condensates of light-matter hybrids known as exciton-polaritons have lacked a direct spin-related control mechanism. Here we demonstrate magnetically tunable exciton-polariton condensation in the antiferromagnetic semiconductor CrSBr, a van der Waals material with strongly linked optical and magnetic properties. Under photoexcitation, CrSBr microwires embedded in an optical cavity show the hallmarks of polariton condensation. The conditions for efficient optical pumping suggest a crucial role of recently discovered surface excitons. Applying an external magnetic field energetically shifts the photoemitting polariton states, enabling direct spin-based control. Our results highlight CrSBr microwires as a powerful platform for exploring magnetically tunable polariton condensates, their directional propagation and their potential for spin-based quantum devices.

HL 39.9 Thu 11:45 POT/0081

Preparation and characterization of CrSBr on opal substrtates — •Jannik Schürmann[1], Aleksandra Lopion[1], Ursula Wurstbauer[1], Alexey V. Scherbakov[2], and Giulia Magnabosco[3] — [1]University of Münster, Münster, Germany — [2]Technische Universität Dortmund, Dortmund, Germany — [3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The magnetic semiconductor Chromium-Sulfur-Bromide (CrSBr) is a highly anistropic van der Waals material. To study the anisotropy of the phononic properties independent from the supporting substrate, the flakes can be detached from it either by suspending it over cavities or by transferring it to a substrate containing closely packed silica spheres (opals). This second approach was already applied to other, nonmagnetic vdW materials such as WSe2 allowing an in-depth pump-probe study of phonons in the material [1]. Accordingly, we transfer mechanically exfoliated CrSBr onto opal substrates using polycarbonate stamps (dry transfer) and thoroughly characterize the properties and qualities of the flakes on opals. Atomic force microscopy confirms that CrSBr is on top of the spheres and partially freestanding. PL and Raman measurements are performed to validate the behavior of the flake in comparison with fully supported one. The decoupled CrSBr flakes on opal substrates are suitable for pump-probe studies of phonon states in CrSBr.
[1] A. Carr et al, ACS Photonics, 11, 1147-1155 (2024) .

HL 39.10 Thu 12:00 POT/0081

Accurate electronic, optical, and magnetic properties of CrSBr via a tuned hybrid functional — •Daniel Hernangómez-Pérez[1], María Camarasa-Gómez[2], Javier Junquera[3], and Ashwin Ramasubramaniam[4] — [1]CIC nanoGUNE BRTA, Donostia, Spain — [2]Centro de Física de Materiales (CFM/MPC), Donostia, Spain — [3]Universidad de Cantabria, Santander, Spain — [4]University of Massachusetts Amherst, USA

CrSBr, a layered antiferromagnet, has attracted attention for its ambient stability, relatively high Néel temperature, and strong exciton-magnon coupling. While experiments have progressed rapidly, computational studies lag due to the high cost of many-body perturbation theory (MBPT). Here, we present a generalized Kohn-Sham density functional approach that accurately reproduces electronic bandstructures, optical spectra, exciton binding energies, and magnon spectra of bulk and few-layer CrSBr at much lower cost than MBPT. Using a minimal two-parameter set tuned to a few benchmarks, we achieve excellent agreement across a broad range of optoelectronic and magnetic properties.
M. Camarasa-Gómez, D. Hernangómez-Pérez, J. Junquera, A. Ramasubramanian (in preparation)

HL 39.11 Thu 12:15 POT/0081

Tunable exchange interaction and hysteresis observed via excitons in a van der Waals antiferromagnet bilayer — •Priyanka Mondal[1], Sonu Verma[2], Wenze Lan[1], Lukas Krelle[1], Ryan Tan[1], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], Akashdeep Kamra[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Physics and Research Center OPTIMAS, Rheinland-Pf\"alzische Technische Universit\"at Kaiserslautern-Landau,Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

Two-dimensional magnets have emerged as key platforms for exploring layer-dependent magnetic phenomena. CrSBr is a recently identified van der Waals magnet with strong excitonic features and layered antiferromagnetic (AFM) order. While pristine bilayers show no magnetic hysteresis, we find that a ~3° twist induces clear hysteresis and can even stabilize a zero-field ferromagnetic state[1]. Field-dependent photoluminescence tracks this behavior through hysteretic exciton energy shifts that match the magnetic configuration. A two-sublattice model explains the response via twist-reduced interlayer exchange, allowing both parallel and antiparallel spin states. The bilayer behaves as an effective monodomain, switching cleanly into the AFM state without forming spin textures. These results highlight twist engineering as a route to programmable magnetic memory in 2D magnets.

[1] P. Mondal et al. arXiv preprint arXiv:2510.08018 (2025).

HL 40: Oxide Semiconductors: Transport and Spectroscopy

Time: Thursday 9:30–12:30 Location: POT/0251

HL 40.1 Thu 9:30 POT/0251

Unraveling metal-induced redox mechanisms on SrTiO3 via combined in-situ laser reflectometry and x-ray photoelectron spectroscopy — •Georg Hoffmann, Shi-Hui Liu, Serkan Sirt, Oliver Bierwagen, and Roman Engel-Herbert — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

SrTiO3 has long served as a key platform for emergent phenomena in perovskite oxides such as polar discontinuity driven two-dimensional electron gases (2DEGs) when interfaced with LaAlO3 [1]. Recently, increasing attention has been brought to 2-DEGs that emerge at SrTiO3 surfaces from redox-reactions induced by amorphous metal deposition on top [2]. Studying these processes, however, requires complex in-situ techniques like photoelectron spectroscopy (XPS) with long measurement cycles. Here, we introduce laser reflectometry (LR) as a complementary technique that enables monitoring of redox-reactions at oxide/metal interfaces. We show that LR in an oxide molecular beam epitaxy setup can distinguish between Al deposition on non-reactive substrates and Al oxidation, e.g. through oxygen scavenging from SrTiO3. Atomic force microscopy, Capacitance-Voltage profiling, and XPS measurements corroborate our findings. Our results demonstrate how LR can guide future investigations of redox-reactions at oxide/metal interfaces. [1] A. Ohtomo, and H. Y. Hwang., Nature 427, 423 (2004). [2] T. Rödel, et al., Adv. Mater. 28, 1976 (2016).

HL 40.2 Thu 9:45 POT/0251

Resonant Raman studies in rutile-Germaniumdioxide — •Kenneth Brandt[1,3], Moritz Meissner[1,3], Zbigniew Galazka[2], Tobias Schultz[2], Markus Wagner[1,3], and Hans Tornatzky[1,3] — [1]Paul-Drude-Institut, Berlin — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Technische Universität Berlin

Ultra-wide bandgap (UWBG) semiconductors are a new research area of interest, with promised applications in power electronics. Germaniumdioxide in the rutile phase (r-GeO_2) has been characterised to be such an UWBG Material with a Bandgap at about 4.5 eV. To be able to create homojunction devices, the material needs to be ambipolar dopable, which poses a challenge for β-Ga_2O_3, as p-type doping has yet to be achieved, while r-GeO_2 is predicted to be ambipolar dopable. Raman measurements show a non typical intensity relationship, in which explicitly the E_g mode does not follow the expected $I \propto \omega^4$ relation of the Raman-Scattering processes but decreases in intensity with higher excitation energies. We are performing resonant Raman studies, with excitation energies ranging from 1.2 eV provided by a tunable Ti:Sa Laser, as well as multiple additional single line Lasers with energies up to 5.1 eV, to investigate the atypical Raman response and electron-phonon coupling.

To quantise the measurements CaF_2 is used as a calibration standard and GaAs is included in the measurement series to compare with literature.

HL 40.3 Thu 10:00 POT/0251

Theoretical Description of a Photo-induced Hidden State in Bismuth Vanadate — •Philip Schwinghammer[1], Verena Streibel[1,2], Frederico Delgado[1], Franziska S. Hegner[1], Viktoria Kunzelmann[1,2], Konrad Merkel[1], Frank Ortmann[1], Ian Sharp[1,2], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Walter Schottky Institute, Technical University of Munich, 85748 Garching, Germany

Bismuth Vanadate has attracted attention in recent years as a promising photoactive material and complex model system. In order to understand new experimental results which show a light-sensitive structure at room temperature, we perform a detailed analysis of the chemical bonding and impact of the exchange-correlation functional. In addition to the use of hybrid functionals, spin-orbit coupling (SOC) stabilizes the experimentally observed monoclinic structure over its high-symmetry tetragonal counterpart. The physical mechanism behind the stabilization is explained through the increase of both covalent and ionic bonding as symmetry breaking causes shortening of select Bi-O bonds. These mechanisms are strongly affected by photo-induced excitation of charge carriers, as the states responsible for the monoclinic distortion are depleted. The alteration of the structure through light may then affect the photo-catalytic efficiencies of the material, as we also find significant differences in the optoelectronic properties of the monoclinic and tetragonal structures.

HL 40.4 Thu 10:15 POT/0251

E-field modulated phase change properties in highly epitaxial VO2 thin film monitored via Raman spectra and IR transmission — •Sonika Singh[1], Rajendra Singh[2], and Ankur Goswami[3] — [1]IIT Delhi, New Delhi, India — [2]IIT Delhi, New Delhi, India — [3]IIT Delhi, New Delhi, India

VO2 is a highly explored smart oxide semiconductor showing metal insulator transition (MIT) at near room temperature ~67 oC. It is observed that optoelectronic properties of highly epitaxial VO2 thin films offer several advantages as compared to polycrystalline film in terms of E-MIT and thermal switching. Here we investigate E-MIT on epitaxial VO2 deposited using PLD technique. Prior to electrical measurement, electrical contacts with 8 *m separation distance were made using Ti/Au metallization. The dual voltage sweep carried over the device demonstrated a high thermal switching ratio (around 30) between high resistive and low resistive state. Furthermore, the dual current sweep was performed on the devices reflected snapback transition signifying uncontrolled and rapid phase transition of VO2. Additionally, E-field dependent Raman spectroscopy revealed modulation of phase transition of VO2 monitored via Raman peaks and triggered via square signal of E-field. These findings suggest that epitaxial thin film of VO2 can be explored for further studies involving modulation of phase change properties via E-field that find direct applications in neuromorphic devices, THz transmissions, thermal switches.

HL 40.5 Thu 10:30 POT/0251

Spatially Resolved Phase Transition and Characterization in Gallium Oxide — Umutcan Bektas[1], Paul Chekhonin[2], Nico Klingner[1], Azat Abdullayev[3], Alexander Azarov[4], René Hübner[1], Zhandos Utegulov[3], Andrej Kuznetsov[4], and •Gregor Hlawacek[1] — [1]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [3]Department of Physics, Nazarbayev University, 010000, Astana, Kazakhstan — [4]Centre for Materials Science and Nanotechnology, University of Oslo, N-0316, Oslo, Norway

In this study, we investigate ion-irradiated β-Ga_2O_3 samples (varying

ions and fluences) alongside α- and κ-Ga_2O_3 thin films. Using focused ion beam (FIB) irradiation, we locally modified the samples under controlled conditions by tuning beam current, size, spacing, scan type, and ion species. Structural changes in the irradiated regions were characterized via electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). Our results demonstrate that ion induced transition to the γ polymorph can be achieved also through FIB irradiation, enabling the fabrication of in-plane polymorph patterns on the nanometer scale. Furthermore, time-domain thermoreflectance (TDTR) measurements further revealed the thermal conductivity of irradiated regions, highlighting opportunities to optimize heat transport in Ga_2O_3 power electronic devices. This research is supported by the tax funds on the basis of the budget passed by the Saxonian state parliament in Germany.

HL 40.6 Thu 10:45 POT/0251

Bandgap, exciton dynamics, and anisotropic thermal transport in rutile-GeO_2 — •Markus R. Wagner[1,2], Luca S. M. Choi[2], Nils Bernhard[2], Pouria Emtenani[2], Felix Nippert[2], Moritz Meissner[1], Hans Tornatzky[1], and Zbigniew Galazka[3] — [1]Paul-Drude-Institut für Festkörperelektronik — [2]Technische Universität Berlin, Institut für Physik und Astronomie — [3]Leibniz-Institut für Kristallzüchtung

Rutile germanium dioxide (r-GeO_2) is a promising ultra-wide bandgap material, predicted to support ambipolar doping and display high thermal and electronic conductivity, making it a strong candidate for power electronics. However, essential aspects of its properties, such as exciton and phonon dynamics as well as the role of defects and impurities, remain only partially explored. Here, we present our recent spectroscopic studies on r-GeO_2. High-resolution spectroscopy of free exciton ground and excited states enables us to determine exciton binding energies and the temperature dependence of the bandgap. Polarization-resolved photoluminescence reveals pronounced differences between near-UV and visible emission bands, which we analyze regarding thermal quenching, recombination dynamics, and charge transfer through temperature- and power-dependent PL, TRPL, and PLE. Using time-domain thermoreflectance down to cryogenic temperatures, we establish the temperatur dependence of thermal conductivity and anisotropy, supported by Boltzmann transport calculations. Finally, polarization-resolved Raman spectroscopy identifies all first-order Raman-active phonons and their relative tensor elements.

15 min. break

HL 40.7 Thu 11:15 POT/0251

MESFETs based on α-$(Al_xGa_{1-x})_2O_3$ thin films — •Sebastian Köpp, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Leipzig, Germany

We present the electrical properties and key parameters of metal-semiconductor field effect transistors (MESFET) on α-$(Al_xGa_{1-x})_2O_3$. The functional thin films were grown by pulsed laser deposition. The transistors were investigated in dependence on the Al content up to x=0.1. The devices exhibit an electrical breakdown field larger than that of comparable transistors on binary α-Ga_2O_3, demonstrating the advantages of the $(Al_xGa_{1-x})_2O_3$ alloy system.
With its ultra-wide bandgap of 5.3 eV to 5.6 eV [1,2] and a high predicted breakdown field of 10 MV/cm [3], α-Ga_2O_3 is a promising material for high-power devices, as well as deep-UV photodetectors. α-Ga_2O_3, being isostructural to aluminium oxide, allows for heteroepitaxial growth on cost-efficient sapphire substrates, and also opens up the option of α-$(Al_xGa_{1-x})_2O_3$ alloys [4], with even higher dielectrical breakdown field than binary Ga_2O_3.

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

HL 40.8 Thu 11:30 POT/0251

Group-III doping study of p-type oxide tin monoxide — •Nicola Gutmann, Georg Hoffmann, Aidan Campbell, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany.

The use of transparent conducting oxides has so far been limited to n-type materials, hindering the development of transparent oxide-based pn-junctions and CMOS devices. In contrast, SnO shows natural p-type conduction with reported hole mobilities up to 21 cm^2/Vs [1] and well-performing p-type transistors demonstrated.

Adjustment of hole concentration by doping with Ga, Na, K and Y has been demonstrated [2]. Al is theoretically predicted to be an n-type dopant [3], which would enable SnO-based pn-homojunctions.

In this work, we comparatively explore doping of suboxide molecular beam epitaxy grown SnO by the group-III elements Al, Ga and In.

[1] M. Minohara et al., J. Phys. Chem. C, vol. 124, no. 2, pp. 1755-1760 (2020).
[2] S. Chae et al., APL Materials, vol. 13, no. 10, p. 101114 (2025).
[3] M. Graužinyte et al., Phys. Rev. Materials, vol. 2, no. 10, p. 104604 (2018).

HL 40.9 Thu 11:45 POT/0251

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

The wide band gap of about 5.3 eV[1] and a high expected breakdown field of up to 10 MV/cm[2], renders the corundum α-phase of Ga_2O_3 interesting for high power electronics. We present lateral p^+n-heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition (PLD) using a two step approach[3]. ZnCoO (ZCO) and NiO deposited by PLD at room temperature were used as p^+-type materials. Further, the influence of a remote oxygen plasma treatment prior to the deposition of the p-type layers on the device performance was investigated. High current rectification ratios of 8.2 (ZCO) and 7.8 (NiO) orders of magnitude at ± 3V were achieved. Additionally, both p-type materials were used as gate materials in the fabrication of α-Ga_2O_3:Zr junction-field-effect-transistors (JFETs), yielding on/off current ratios of more than 9 orders of magnitude and sub-threshold-swings down to 119 mV/dec. Furthermore, breakdown was detected at drain voltages of up to 476 V which is estimated to a field of 1.7 MV/cm [4].

[1] A. Hassa et.al., J.Phys. D: Appl. Phys. **54**, 223001 (2021)
[2] M. Biswas et al., APL Mater. **10**, 060701 (2022)
[3] S. Vogt et al., Phys. Status Solidi A, **220** 2200721 (2023)
[4] P. Bokemeyer et al.,Phys. Status Solidi RRL, 2400388 (2025)

HL 40.10 Thu 12:00 POT/0251

Defect-Induced Resistive Switching in Titanate-based Perovskites — •Parrydeep Kaur Sachdeva[1], Wahib Aggoune[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI of MPG, Berlin — [2]Institut für Physik and CSMB, Humboldt-Universität zu Berlin, Berlin

Perovskites possess strong potential for exhibiting ferroelectric resistive switching (RS), a functionality recently realized yet not understood in titanate perovskites [1]. Controlled deviation from stoichiometry has revealed high RS, indicating a defect-mediated origin. Using hybrid functional DFT calculations, we show that the Ti antisite defect (Ti-interstitial with Ca-vacancy) can induce ferroelectricity in $CaTiO_3$ which is an incipient ferroelectric, stabilized in a non-polar state by strong octahedral tilts. The Ti-interstitial atom breaks this balance by its off-center displacement and induces a local polarization. This polarization is switchable between different off-center positions of the defect, with energy barriers in the range of 0.25 eV. Additionally, the Ti antisite defect gives rise to mid-gap states, with a charge density mainly localized around the Ti-interstitial atom. Switching the defect between equivalent off-center positions switches the polarization direction and alters the spatial distribution of the charge state. This can influence the material's overall response under external stimuli. These results are discussed with respect to the experimentally observed resistive switching in titanate-based perovskites [1], as reported by Leibniz-Institut für Kristallzüchtung (IKZ) Berlin.

[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 40.11 Thu 12:15 POT/0251

ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type transparent conducting oxides — •Daniel Fritsch — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

ZnM_2O_4 (M = Co, Rh, Ir) spinels are under investigation as potential p-type transparent conducting oxides (TCOs) [1]. Here we extend our previous investigation of $ZnRh_2O_4$ into the whole series of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

To this end, we perform *first-principles* calculations based on density functional theory employing a recently developed *self-consistent* hybrid exchange and correlation functional [2], and compare the results to more standard HSE06 hybrid functional calculations. In order to judge the results on the electronic and optical properties, additional calculations based on many-body perturbation theory, i.e. G_0W_0 calculations, have been performed and allow for a more detailed analysis of the applicability of ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type TCOs.

The obtained structural, electronic, and optical properties will be discussed alongside earlier experimental and theoretical investigations, and will open a pathway to potential applications of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

[1] D. Fritsch, Electron. Mater. **2**, 504 (2021).
[2] D. Fritsch, B. Morgan, and A. Walsh, Nanoscale Res. Lett. **12**, 19 (2017).

HL 41: Quantum Dots and Point Contacts (joint session TT/HL)

Time: Thursday 11:00–12:45 Location: HSZ/0101

HL 41.1 Thu 11:00 HSZ/0101

Mapping dissipation in a quantum dot junction — •Johannes Höfer[1], Subhomoy Haldar[2], Ville Maisi[2], Hervé Courtois[1], and Clemens B. Winkelmann[1,3] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 25 rue des Martyrs, Grenoble, France — [2]NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden — [3]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, Grenoble, France

Characterization of quantum devices relies primarily on electrical properties. It is usually assumed that all parts of the device remain at the same temperature, but the inevitable presence of local dissipation can lead to significant deviations and degrade device performance [1].

Here, we present simultaneous measurement of the current through a quantum dot junction as well as the dissipation generated by the current. To this end, we thermally isolate the drain contact of an epitaxially defined quantum dot in an InAs nanowire. The electron temperature is measured via the zero-bias conductance of a Josephson junction [2]. Due to the energy-selective transport through a single quantum level, we can tune the dissipation solely with a gate voltage, while keeping both the current and voltage across the dot constant.

The presented device enables future investigations of local dissipation in nanoscale devices, e.g. for mitigation of detrimental heating effects, as well as implementations of proposed experiments in the field of quantum thermodynamics.

[1] S.G.J. Philips et al., Nature 609 (2022) 919
[2] B. Karimi, & J.P. Pekola, Phys. Rev. Applied 10 (2018) 054048

HL 41.2 Thu 11:15 HSZ/0101

Lindblad-based linear response of hybrid semiconductor-superconductor devices — •Tobias Kuhn, Raffael L. Klees, and Monica Benito — Augsburg University, Augsburg, Germany

The field of hybrid semiconductor-superconductor quantum dots is pushing towards the development of functional devices that harness the advantages of both worlds. Their complexity calls for a complete theoretical framework to understand responses to different probe fields and dissipation induced by the environment. We present a Lindblad-based linear response formalism, built upon the framework introduced in Ref. [1]. It captures not only the inherently multi-level nature of these devices but also their probe-readout flexibility and non-unitary effects of the finite-frequency response. We exemplify the framework using quantum dot based Kitaev chain setups which are promising candidates for topologically protected qubits [2,3].

[1] L. Peri, M. Benito, C. J. B. Ford, and M. F. Gonzalez-Zalba, npj Quantum Inf **10**, 1 (2024)
[2] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012)
[3] D.M.Pino, R.S.Souto, R.Aguado, Phys. Rev. B**109**, 075101 (2024)

HL 41.3 Thu 11:30 HSZ/0101

Dynamics of strong correlations of a hybrid quantum dot system with superconducting and ferromagnetic electrodes — •Antoni Jankiewicz, Kacper Wrześniewski, and Ireneusz Weymann — Institute of Spintronics and Quantum Information, Adam Mickiewicz University, Poznań, Poland

We theoretically explore the non-equilibrium dynamics of a quantum dot coupled to superconducting and ferromagnetic electrodes. This hybrid setup offers a rich platform to investigate the interplay between strong correlations, superconductivity, and ferromagnetism at the nanoscale. To perform the analysis we employ the numerical renormalization group and its time-dependent extension. These methods enable us to capture the subtle nature of dynamical quantum phase transitions induced by abrupt changes in Hamiltonian parameters, known as quantum quenches. Such transitions are crucial for understanding the stability and evolution of many-body states in response to external perturbations.

The aim of this work is to examine the competition between the superconducting pairing and the dot's spin. For that, we determine the time dependence of key observables, including the dot's spin and the on-dot pairing correlations. We demonstrate that these quantities reveal the competing character of correlations as they oscillate in counter-phase. Furthermore, we also analyze the dynamical quantum phase transitions in the system by determining the Loschmidt echo and the return function, which provide direct measures of the system's sensitivity to quenches.

HL 41.4 Thu 11:45 HSZ/0101

Tunneling resonances through periodically driven quantum dots — •Jan Mathis Giesen, Daniel Weber, and Sebastian Eggert — RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

We consider a general setup of transport through a time-periodically driven quantum dot using Floquet theory. An analytic non-equilibrium solution of the problem is developed which allows the analytic prediction and analysis of the tunneling amplitudes as a function of frequency, driving amplitude, and energy levels on the dot. One main result is the discovery of a previously unknown resonant switching effect, where a very small control signal on a weakly connected quantum dot can induce perfect transmission. This opens the door for the design of novel efficient nano-electronic devices. The results are also relevant for corresponding setups using magnonic systems, photonic waveguides, or ultra-cold gases in optical lattices.

HL 41.5 Thu 12:00 HSZ/0101

Spectroscopic-imaging Coulomb blockade microscopy — Junho Bang[1], Byeongin Lee[1], Hankyu Lee[1], •Jianfeng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We use scanning tunneling microscopy (STM) to directly visualize Coulomb blockade (CB) phenomena in the double-barrier tunnel junction formed between the STM tip and crystalline indium nanoislands on semiconducting black phosphorus. Spatially resolved tunneling spectra reveal bias-dependent dispersions of CB peaks across individual nanoislands. Strikingly, the trajectories of CB peaks exhibit twofold asymmetries: (i) their curvatures reverse sign across a nonzero bias offset, and (ii) the trajectories lack mirror symmetry about this bias offset. Simulations based on orthodox theory faithfully reproduce both asymmetries, which we trace to work-function mismatches at (i) the island-tip and (ii) the island-substrate interfaces, respectively. These results establish spectroscopic-imaging Coulomb-blockade microscopy as a quantitative probe of junction parameters, offering a pathway for diagnosing and optimizing single-electron charge sensors relevant to quantum-computing architectures.

HL 41.6 Thu 12:15 HSZ/0101

Electromigrated palladium nano-contacts: formation of atomic contacts and non linear current-voltage characteristics — •Samanwita Biswas[1], Thomas Hultzsch[1], Marcel Strohmeier[2], Elke Scheer[2], and Regina Hoffmann-Vogel[1] — [1]Institute of Physics and Astronomy, University of Potsdam — [2]Department of Physics, University of Konstanz

We investigate the electronic transport properties of atomic-size Pd contacts fabricated by electromigration (EM) of lithographically defined nano-constrictions, at room temperature in different environ-

ments. In particular we study changes in the conductance upon EM with a focus on possible shell effects [1]. By systematic analysis of a large number of data sets in the conductance range up to $\sim 10G_0$ (with the conductance quantum $G_0 = 2e^2/h$), we identify preferential conductance values and compare these with the ones expected for shell closure in multivalent metals. For contacts with $G \lesssim 5G_0$, the current-voltage characteristics often become nonlinear on a scale of few 100mV; we discuss this observation with respect to structural changes during the thinning process of EM. By monitoring the smallest conductances, we often identify a decrement of resistance inside a cycle, opposite to the overall trend, indicating the transition to the ballistic regime. Our results suggest that metallic few atomic contacts of Pd, despite being more reactive than noble metals, can be stabilized even at room temperature.

[1] Mares & van Ruitenbeek, Phys. Rev. B 72, 205402 (2005)

HL 41.7 Thu 12:30 HSZ/0101

Readout of multi-level quantum geometry from electronic transport — •Raffael L. Klees and Mónica Benito — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

The quantum geometric tensor (QGT) of a quantum system in a given parameter space captures both the geometry of the state manifold and the topology of the system [1]. While the local QGT elements have been successfully measured in various platforms, the challenge of detecting them in electronic transport systems − such as tunnel or molecular junctions − has yet to be resolved. To fill this gap, we propose a measurement protocol based on weak and resonant parameter modulations [2], and theoretically demonstrate how the local QGT in such systems can be directly probed from changes of the tunnel conductance [3]. This approach enables the measurement of both geometrical and topological features of quantum states in a broad class of transport-based quantum systems.

[1] M. Kolodrubetz *et al.*, Phys. Rep. **697**, 1 (2017)
[2] T. Ozawa and N. Goldman, Phys. Rev. B **97**, 201117(R) (2018)
[3] R. L. Klees and M. Benito, arXiv:2508.08239 (2025)

HL 42: Nitrides III – Emerging thin films and electrochemistry

Time: Thursday 11:15–12:45 Location: POT/0006

Invited Talk HL 42.1 Thu 11:15 POT/0006

Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion — •Verena Streibel[1,2], Laura I. Wagner[1,2], Elise Sirotti[1,2], David A. Egger[2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Transition metal nitride thin films are emerging as promising materials for (photo)electrochemical applications. However, their synthesis and defect control remain challenging. Here, we use reactive co-sputtering to synthesize and engineer nitride thin films with precise control over composition and doping in the Ti-Ta-N,[1] Zr-Ta-N,[2,3] and Hf-Ta-N materials space. Starting from orthorhombic Ta_3N_5, we show that substitutional Ti doping improves photoconversion efficiency by modulating defects and recombination dynamics. While high Ti doping forms a secondary TiN phase, Zr and Hf yield tunable solid solutions in the Zr-Ta-N-(O) and Hf-Ta-N-(O) systems, exhibiting bandgap modulation and large refractive indices. Notably, a new bixbyite-type ternary compound, $ZrTaN_3$, forms at a 1:1 Zr:Ta ratio, showing strong visible light absorption and photoanodic activity. DFT calculations reveal a tunable direct bandgap driven by cation ordering.[3] Our findings establish composition engineering as a key strategy for tailoring band structure and charge transport in emerging nitride semiconductors.

[1] Wagner, L.I. et al., Adv. Funct. Mater. 2024, 34, 2306539.
[2] Wagner, L.I. et al., Adv. Mater. Interfaces 2025, 12, 2400745.
[3] Sirotti, E. et al., Adv. Energy Mater. 2024, 202402540.

HL 42.2 Thu 11:45 POT/0006

Analysis of the interface properties of cubic nitride thin films grown on 3C-SiC/Si templates using electrochemical impedance spectroscopy — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor material for a variety of applications, such as high-power electronics or optoelectronic devices. High quality c-GaN can successfully be grown by molecular beam epiatxy on 3C-SiC/Si templates making use of a c-AlN buffer layer, which accommodates lattice mismatch between c-GaN and the 3C-SiC template. A reliable characterization of the interface properties as well as the electrical transport properties of c-GaN is crucial for optimizing the thin film growth as well as for designing advanced functional devices. In this work we employ electrochemical impedance spectroscopy (EIS) for characterizing the transport throught c-GaN/AlN/3C-SiC/Si sample structures with different c-GaN thicknesses and for analyzing the properties of the interface, such as the trap density.

HL 42.3 Thu 12:00 POT/0006

Investigating Charge Transport Limitations in $LaTiO_2N$ Thin Films for Photoelectrochemical Water Splitting — •Oliver Brune[1,2], Gabriel Grötzner[1,2], Katarina S. Flashar[1,2], Saswati Santra[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Photoelectrochemical water splitting offers a sustainable route to hydrogen production. On the photoanode side, $LaTiO_2N$ is a promising candidate due to its visible-light absorption, favorable band alignment and n-type semiconducting properties. However, its performance is limited by inefficient charge transport, the origin of which remains unclear. In this work, we synthesize $LaTiO_2N$ thin films by spin coating and reactive sputter deposition, both followed by ammonia annealing, yielding films with controlled structure and composition as confirmed by XRD and ERDA/RBS. Synchrotron-based XAS, XPS, UV-Vis spectroscopy, and PEC measurements reveal that a larger degree of nitridation in $LaTiO_2N$ correlates with higher short-range order and crystallinity, a decreasing bandgap, and an increase in photocurrent density. To elucidate charge transport mechanisms and carrier dynamics, we use Hall effect and temperature-dependent photocurrent measurements. Our findings establish a direct link between synthesis parameters, defect chemistry, and charge-carrier dynamics in $LaTiO_2N$, providing a foundation for overcoming transport limitations in oxynitride-based photoanodes for solar hydrogen production.

HL 42.4 Thu 12:15 POT/0006

Epitaxial YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy — Yitong Chen[1,2], •Anna Meléndez Sans[1,3], Shin-ichi Kimura[2,4,5], Liu Hao Tjeng[1], and Simone Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, Graduate School of Science, The University of Osaka, Toyonaka, Japan — [3]Institut de Ciència de Materials de Barcelona, Bellaterra, Spain — [4]Graduate School of Frontier Biosciences, The University of Osaka, Suita, Japan — [5]Institute for Molecular Science, Okazaki, Japan

Rare-earth mononitrides display interesting magnetic and semiconducting properties due to the strongly correlated and localized $4f$ electrons. However, extreme air sensitivity and poor stoichiometry hindered research on bulk samples when they were first discovered. Modern advancements in UHV-based thin film growth techniques have opened the possibility to synthesize and study high quality samples.

Unlike most of the rare-earths, which can break the molecular nitrogen bond, Yb does not react with nitrogen gas and therefore requires an activated nitrogen source for the synthesis of YbN.

Here we present our growth study on YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy, using different substrates (MgO and $LaAlO_3$) and growth conditions. The films were characterized *in situ* with photoelectron spectroscopy, confirming their semiconducting character and the Yb valence as 3+. Photon-energy dependence of the valence band spectra revealed a significant hybridization of the Yb $4f$ and N $2p$ states.

HL 42.5 Thu 12:30 POT/0006

Novel TbTa(O,N)$_3$ perovskite oxynitride for photoelectrochemical energy conversion — •Aleksandr Kochergov[1,2], Gabriel Grötzner[1,2], Oliver Brune[1,2], Frans Munnik[3], Saswati Santra[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Perovskite oxynitride semiconductors have emerged as promising candidates for photoelectrochemical (PEC) water splitting, given their smaller band gaps ($\sim$ 2 eV) compared to more extensively studied metal oxides. Previous studies show that in rare-earth lanthanide tantalum perovskite oxynitrides, PEC photocurrent density increases with the increment of the A-site cation atomic number [1]. However, no studies have investigated A-site cations heavier than gadolinium (Gd). This work presents a method for synthesizing the novel perovskite oxynitride TbTa(O,N)$_3$ as thin film via spin coating followed by a sequential two-step annealing procedure in air and ammonia. X-ray diffraction shows that proper NH_3 annealing conditions are crucial for obtaining the TbTa(O,N)$_3$ perovskite structure. The resulting films are investigated for their structural, compositional, and optoelectronic properties. The results suggest a 2.3 eV band gap and n-type conductivity. Given these favorable properties, the viability of TbTa(O,N)$_3$ as photoanode is evaluated.

[1] Zou, Qi, et al., J. Am. Chem. Soc. 2024, 146, 28182-28189

HL 43: Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)

We are organizing an Excursion and Network-Event to Infineon Dresden AG.
Only for registered and selected participants.
Please register until latest February 12th here: https://www.icams.de/news-events/events/registration-infineon/?api=561b8d7cfcb678e9f0938830d78cf979

Time: Thursday 13:30–17:00 Location: Infineon

Only for registered and selected participants.

HL 44: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)

Time: Thursday 15:00–17:45 Location: HSZ/0204

HL 44.1 Thu 15:00 HSZ/0204

Linearized augmented plane waves for low-dimensional materials — •Andris Gulans, Ernests Jansons, and Janis Uzulis — University of Latvia, Riga, Latvia

We address the challenge of efficient yet highly precise density-functional theory calculations of low-dimensional materials and present a set of tools and algorithms specific to linearized augmented plane waves (LAPW) that is implemented in the electronic-structure code `exciting`. First, we discuss our iterative eigensolver compatible with local and hybrid functionals. It is an extension of Davidson*s algorithm and does not require explicit Hamiltonian construction while overcoming difficulties associated with high condition numbers. The second important ingredient is the adaptively compressed exchange that represents the non-local (screened) Fock exchange via a low-rank approximation. This approach enables computational complexity as low as $O(N^3 \log N)$ floating-point operations (FLOPs) with N being the number of atoms. It is a novel feature in hybrid functional calculations using LAPW as the standard approaches require $O(N^4)$ FLOPs. Finally, we introduce a cylindrical cutoff for the Coulomb interaction for handling the $q = 0$ singularity.

HL 44.2 Thu 15:15 HSZ/0204

Graphene-Enabled Mott–Metal Transition in Silicon Dangling Bonds — •Niclas Tilgner[1], Siheon Ryee[2], Zamin Mamiyev[1], Philip Schädlich[1], Christoph Tegenkamp[1], Tim O. Wehling[2], and Thomas Seyller[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]I. Institute of Theoretical Physics, University of Hamburg, Germany

Controlling emergent electronic phases in materials with strong Coulomb interactions remains a central challenge in condensed matter physics. Adatom lattices on semiconducting surfaces provide prototypical platforms for exploring such correlated phenomena. Recent advances have facilitated the synthesis of 2D Mott insulators in proximity to graphene (N. Tilgner et al 2025 2D Mater. 12 045022). Here, we demonstrate that alkali adsorption on a graphene/Si/SiC(0001) heterostructure – where the Si layer hosts correlated dangling bonds – enables controlled charge transfer to the Mott insulator. Beyond a critical carrier concentration, we observe a sudden collapse of the Mott gap, indicating a transition to a correlated metallic phase. Our results point to a finite proximity coupling between the Mott layer and graphene, as recently suggested by a theoretical study (N. Witt et al 2025 arXiv:2503.03700), which gives rise to nonlocal dynamical screening beyond simple electrostatics and provides a natural pathway for the observed phase transition.

HL 44.3 Thu 15:30 HSZ/0204

From self-consistent DFT+DMFT to the two-particle level: Magnetic phase diagram of X:SiC(111) — •Lukas Bongardt[1,2], Niklas Enderlein[3], Giorgio Sangiovanni[4], Philipp Hansmann[3,5], and Henri Menke[1] — [1]Max Planck Computing and Data Facility — [2]Technical University of Munich — [3]FAU Erlangen — [4]Universität Würzburg — [5]University of Iceland, Reykjavík

Recently we have proposed a novel and versatile platform to realize a two-band Hubbard model with massless Dirac fermions and flat bands hosting strong correlations by depositing three different species of transition-metal adatoms on semiconductor surfaces (arXiv:2410.17165). Using state-of-the-art DFT+DMFT calculations we investigated the spectral properties of X:3C-SiC(111) (X = Ti, V, Cr). Due to the presence of well-defined Dirac cones and flat bands, indicating the potential for realizing topological and correlated phases, we identify transition-metal adatoms on SiC as a possible platform for exploring the interplay of correlations, topology, and magnetism in two-dimensional materials.
In this work, we explore the magnetic phase diagram of these systems within DMFT by calculating the generalized two-particle vertex and using it to solve the Bethe-Salpeter equation for the generalized susceptibility. This gives us a fully orbital-, spin-, and most importantly momentum-dependent susceptibility which carries the information about the ordering wave vector and is experimentally accessible through various techniques.

HL 44.4 Thu 15:45 HSZ/0204

Cr 3*d* Orbital Hybridization and Electronic Structure in the Layered Magnetic Semiconductor CrPS$_4$ — •Lasse Sternemann[1], David Maximilian Janas[1], Richard Leven[1], Eshan Banerjee[2], Jonah Elias Nitschke[1], Marco Marino[1], Leon Becker[3], Ahmet Can Ademoglu[1], Frithjof Anders[1], Stefan Tappertzhofen[3], and Mirko Cinchetti[1] — [1]TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — [2]Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom — [3]TU Dortmund University, Department of Electrical Engineering and Information Technology, 44227 Dortmund, Germany

Despite its promising spintronic and magneto-optical characteristics, the electronic band structure of the van der Waals magnetic semiconductor $CrPS_4$ is still unknown. Here, we report angle-resolved photoemission spectroscopy measurements of its band structure in the para- and antiferromagnetic phase, complemented by DFT+U calculations.

Theoretical results reveal dominating Cr 3*d* and S 3*p* contributions to the valence band and a ligand-to-metal charge-transfer band gap. Crystal field split Cr 3*d* orbitals display distinct hybridization regimes with S 3*p* orbitals: t_{2g} orbitals are only weakly affected by hybridization, while e_g states experience a 4 eV anti-bonding/bonding splitting with S-mixing relaxing dipole selection rules, otherwise darkening optical *d*-*d* transitions. These findings establish the ground state electronic and orbital structure of $CrPS_4$ and provide essential benchmarks for understanding its optical and magnetic responses.

HL 44.5 Thu 16:00 HSZ/0204

Spectroscopic Investigation of the Ni Valence States in $NiTe_2$ — •Tassaphon Tirasutt[1], Sheng-Huai Chen[1], Alexander C. Komarek[1], Chun-Fu Chang[1], Yu-Chieh Ku[2], Po-Yu Cho[3], Chun Sum Brian Pang[4], Mizuki Furo[5], Naoki Ito[5], Ulrich Burkhardt[1], Simone G. Altendorf[1], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]The University of British Columbia, Vancouver, Canada — [5]Osaka Metropolitan University, Osaka, Japan

Nickel-based transition metal compounds exhibit a wide range of properties arising from the strongly correlated *d* electrons. In this study, we investigate $NiTe_2$, a layered transition-metal dichalcogenide with reported type-II Dirac semimetallic properties. While its topological nature has been the focus of interest, the fundamental question of the properties of the Ni ions in $NiTe_2$ has rarely been discussed. We address this issue using soft X-ray core-level and valence-band photoelectron spectroscopy, as well as Ni-$L_{2,3}$ absorption spectroscopy, combined with a theoretical approach using LDA+DMFT. Our findings provide insights into the Ni 3*d* occupation and degree of correlation of the Ni in a metallic ligand bath of the $NiTe_2$ system.

HL 44.6 Thu 16:15 HSZ/0204

TMDC surfaces as scattering targets in spin-polarization detectors: A case study of MoS_2 — •Christoph Angrick[1], Annika Henriksen[1], Nicole Edossa[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Spin-polarization detectors are employed in photoemission experiments to reveal the spin texture of electronic states. One well-proven approach is based on the VLEED process, where the spin-dependent electron reflection from targets influenced by exchange and/or spin-orbit interaction is used. The suitability of a target must be investigated beforehand [1,2]. In this talk, a first impression of TMDC-based detectors is given [3]. The spin-dependent electron reflectivity of spin-orbit-influenced MoS_2 is measured over a wide range of incident energies and angles for the following samples: a single layer of MoS_2 on Au(111) and cleaved MoS_2 single-crystal surfaces. On the basis of the resulting maps for the electron reflectivity, Sherman function, and figure of merit, promising features of MoS_2 for use in spin-polarization detection are discussed.

[1] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).
[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[3] Angrick *et al.*, Phys. Rev. B, accepted for publication (2025).

HL 44.7 Thu 16:30 HSZ/0204

Efficient GW calculations for metals from an accurate ab initio polarizability: the case of doped MoS2 monolayer — •Giacomo Sesti[1], Pino D'Amico[1], Alberto Guandalini[2], Claudia Cardoso[1], Andrea Ferretti[1], and Daniele Varsano[1] — [1]CNR-NANO, Modena, Italy — [2]Università di Roma La Sapienza, Roma, Italy

Many-body perturbation theory in the GW approximation has proved very successful for the calculation of quasiparticle (QP) band structures of semiconductors. QP corrections are less significant in metals and are typically disregarded for the computational cost involved. Also, GW calculations of metals suffer of specific methodological challenges to properly treat the screening. This is typically solved under the addiction of a Drude term, that however is inadequate at low dimensionalities[1]. Furtherly, even for metals, QP corrections become more relevant at lower dimensionalites.

Here, we present GW calculations of QPs for doped MoS_2 monolayer showing excellent agreement with experimental ARPES measurements[2]. Such an unprecedented agreement has been possible thanks to the W-av method, which combines a Monte Carlo integration with interpolation approaches. This technique originally developed for 2D semiconductors[3] is here extended to the metallic case.

1) Champagne et al. NanoLett. 23.10 (2023)
2) Liu et al. PRL. 122 (2019)
3) Guandalini et al., npj Computational Materials, 9 (2023)

HL 44.8 Thu 16:45 HSZ/0204

Ultrafast Momentum Dependent Relaxation Dynamics in $TbTe_3$ — •Florian Denizer[1], Noah Meyer[2,3], Anisha Singh[3], Ian R. Fisher[3], Uwe Bovensiepen[1], Zhi-Xun Shen[2,3], and Patrick S. Kirchmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University — [3]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University

Rare-earth tritellurides (RTe_3) form charge density waves (CDW) due to electronic instabilities at the Fermi-surface, because of an anisotropy of the crystal lattice between the two major in-plane crystal axes *a* and *c*. Unoccupied electronic states can be populated by ultrafast laser excitation. Electronic relaxation and coherent vibrational modes including the amplitude mode have been investigated by time and angle resolved photoelectron spectroscopy (*tr*-ARPES). Among the manifold of laser-driven processes, the one that is responsible for the electronic instability has not yet been identified. With this objective in mind we perform a *tr*-ARPES experiment on $TbTe_3$ and investigate the momentum transfer along the a- and the c-axis as a function of excitation strength. At sufficiently low pump fluence below $F = 0.3$ mJ/cm^2 we identify (quasi-)elastic scattering in the vicinity of the Fermi surface. In the talk we will discuss isotropic defect-induced elastic scattering and directed quasi-elastic scattering determined by the nesting vector. Funding through the DFG within SFB 1242 and through the DOE is gratefully acknowledged.

HL 44.9 Thu 17:00 HSZ/0204

Unconventional Topological Superconductivity in CrCl3/NbSe2 heterostructures — •Souvik Das[1], Benjamin Zhou[2,3], Anshuman Padhi[1], Jing-Rong Ji[1], Niclas Heinsdorf[2,3], Prajwal Rigvedi[1], Tianzhe Chen[1], Weibin Li[4], Pierluigi Gargiani[4], Manuel Valvidares[4], Marcel Franz[2,3], Banabir Pal[1], and Stuart S.P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [4]ALBA Synchrotron Light Source, Barcelona, Spain

Topological p-wave superconductors can host non-Abelian particles useful for fault-tolerant quantum computing. Here we report experimental evidence of unconventional topological superconductivity in a heterostructure of monolayer, in-plane ferromagnetic CrCl3 islands on superconducting NbSe2. STM measurements show that, despite CrCl3 being ferromagnetic, the interfacial superconducting gap is more robust against out-of-plane magnetic fields than the s-wave gap of NbSe2, indicating unconventional pairing. We also find enhanced zero-energy states along CrCl3 island edges, consistent with the presence of edge modes. Theory suggests these features arise from an intrinsic helical p-wave state stabilized by interfacial Rashba spin-orbit coupling. This demonstrates a new route to create topological superconductivity via interface engineering.

HL 44.10 Thu 17:15 HSZ/0204

Structural and Electronic Properties of CrSBr Nanoribbons: Insights from First-Principles Calculations — •Daniil Kruklinskii, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Experiments show that exfoliated CrSBr flakes naturally form nanoribbons along a specific crystallographic direction, and similar structures can be fabricated using an electron beam in the TEM as a cutting tool. Here, we employ density functional theory calculations to systematically investigate the stability as well as electronic and magnetic properties of CrSBr nanoribbons. Our results indicate that nanoribbons oriented along one of the two major crystallographic directions are the most stable under typical growth and exfoliation conditions and remain semiconducting, exhibiting pronounced electron-hole separation between the VBM and CBM. In contrast, nanoribbons in the perpendicular direction display a substantially reduced band gap due to strongly localized edge states. Both orientations retain strongly spin-

polarized band-edge states near the Fermi level and show only a weak dependence of the band gap on ribbon width. Using *ab initio* molecular dynamics simulations, we further demonstrate that electron-beam irradiation with energies of at least 200 keV can facilitate the fabrication of nanoribbons directly from pristine monolayer CrSBr, favouring the formation of diagonal nanoribbons. These diagonal ribbons are metallic, in contrast to the monolayer, and host a high density of majority-spin edge states, giving rise to pseudo-half-metallic transport.

HL 44.11 Thu 17:30 HSZ/0204

Band-selective coherent phonon-driven band renormalization in 1T-$MoTe_2$ — •Carl Jensen[1], Christopher Emeis[2], Stephan Jauernik[1], Petra Hein[1], Fabio Caruso[2], and Michael Bauer[1,3] — [1]nstitute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Understanding the coupling between coherent phonons and the electronic system is crucial for controlling nonequilibrium properties in solids. Here, we investigate mode- and band-selective electron-phonon coupling in centrosymmetric 1T-$MoTe_2$ using time- and angle-resolved photoemission spectroscopy combined with frequency-domain analysis (FDARPES). Femtosecond near-infrared pulses excite coherent Ag-symmetric phonon modes at 2.34 THz, 3.34 THz, and 3.86 THz, which manifest as oscillatory modulations in photoemission intensity and binding energy across the valence bands. Pixel-wise Fourier analysis, based on a recently developed methodology [1], reveals pronounced band selectivity with distinct coupling strengths for different electronic states and phonon modes, enabling the evaluation of band-renormalization amplitudes in the few-meV range. Ab initio calculations using DFT/DFPT qualitatively reproduce the experimentally observed coupling patterns and relative trends, demonstrating the capability of combined experimental and theoretical approaches to resolve ultrafast electron-phonon interactions in quantum materials.

[1] N. Gauthier, H. Soifer, J.A. Sobota, H. Pfau, E. J. Sie, A. M. Lindenberg, Z.-X. Shen, P. S. Kirchmann, Rev. Sci. Instrum. 96 (2025)

HL 45: Perovskite and Photovoltaics: Spectroscopy

Time: Thursday 15:00–17:15 Location: POT/0006

HL 45.1 Thu 15:00 POT/0006

The influence of air and light exposure on alkali-metal doped Cu(In,Ga)Se_2 absorber materials measured with in-situ TRPL and XPS — •P. Stötzner, S. Sobisch, A. Stauffenberg, H. Kempa, R. Scheer, and S. Förster — Martin-Luther-Universität Halle-Wittenberg, Germany

Copper indium gallium diselenide (Cu(In,Ga)Se_2/CIGSe) is a promising thin-film solar cell absorber. Alkali-metal doping, especially in combination with heavy alkali metals, enhances solar cell efficiencies. However, air and light exposure (ALE) of the absorber reduces the solar cell efficiency. This is a result of the diffusion of sodium and oxygen toward the absorber surface, which is accompanied by a degradation of the charge-carrier lifetime of doped CIGSe absorbers [1,2].

Here, we study the ALE effect for CIGSe doped with K and cominations of Na and K as well as Na and Rb. Our studies combine X-ray photoelectron spectroscopy (XPS) and in-situ time-resolved photoluminescence (TRPL) conducted in one ultrahigh vacuum system, addressing changes in the chemical composition and charge-carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.

We find that the charge-carrier lifetime of non-doped absorbers is unaffected by ALE and all alkali-metal doped absorbers degrade due to ALE. XPS shows that the most heaviest alkali metal present and oxygen are accumulated at the surface. While this effect is reversable over time, the degradation of the charge-carrier lifetime is permanent.

[1] DOI: 10.1063/1.4992116 [2] DOI: 10.1002/pip.3041

HL 45.2 Thu 15:15 POT/0006

Thermal Broadening Statistics of Photoluminescence in Tunable Lead Halide Perovskite Nanocrystals — •Luca B. Reim, Leo Luber, and Alexander S. Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich

Halide perovskite nanocrystals (NCs) exhibit excellent optoelectronic properties, including high quantum yields and composition-dependent, narrow photoluminescence (PL) that critically depend on control over NC size and uniformity. Understanding the mechanisms governing PL linewidths is therefore essential for evaluating material quality and device performance.

We synthesized size-tunable $CsPbBr_3$ nanocubes under ambient conditions using machine-learning-optimized reaction protocols.[1] The NCs were drop-cast onto substrates and investigated via temperature-dependent PL spectroscopy in a closed-cycle cryostat from 9-300 K. To quantitatively analyze the spectral evolution, we applied a novel fitting approach that enables the extraction of size dispersion, temperature-dependent exciton populations, and signatures of the local energetic environment. The latter is strongly influenced by nanocrystal quality and ligand coverage and provides a sensitive probe of inhomogeneous broadening mechanisms.

These results offer detailed insight into the fundamental limits of emission linewidths in perovskite NCs and support the targeted optimization of materials for optoelectronic applications such as LEDs.

[1] N. A. Henke, et al., Adv. Mater. 2025, e09472.

HL 45.3 Thu 15:30 POT/0006

Investigation on the efficiency limiting processes of 3C-SiC photoelectrodes using intensity modulated techniques. — •Marius Wasem[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Cubic silicon carbide (3C-SiC) is a compelling photoelectrode for photoelectrochemical water splitting due to its near-ideal band gap energy and excellent chemical stability. Here, we present the characterization of the photoelectrochemical response of epitaxially grown n- and p-type 3C-SiC using different electrochemical methods. A pH neutral phosphate buffer solution was used as electrolyte. The suitable operating conditions, such as potential range and light intensity, were determined using chopped light voltammetry. Insights of the charge carrier dynamics were gained by combining electrochemical impedance spectroscopy (EIS), intensity-modulated photocurrent spectroscopy (IMPS) and intensity-modulated photovoltage spectroscopy (IMVS). While EIS is a common and widely used method, the latter two methods are rarely discussed in the photoelectrochemical community. Here we show how a combination of all three methods enables the differentiation and quantification of key processes (recombination processes, surface effects, charge carrier lifetime) to validate the efficiency of 3C-SiC photoelectrodes.

HL 45.4 Thu 15:45 POT/0006

Nano-sensing of AC-Fields with Perovskite Quantum Dots and Electro-Switching of Luminescence — •Emanuel Eckl[1], Fabian Brütting[1], Moritz B. Heindl[1], Maryna Bodnarchuk[2], Mariia Svyrydenko[2], Maksym Kovalenko[2], and Georg Herink[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]ETH Zürich, Zürich, Switzerland

Perovskite quantum dots (PQDs) currently attract significant research interest, particularly owing to their broad tunability of optoelectronic properties with applications in energy conversion, solid-state lighting and sensing technologies.

In this study, we investigate the potential of PQDs as nano-sensors for transient electric fields up to multi-Terahertz (THz) frequencies [1]. Combining electro-absorption, lifetime and photoluminescence measurements of inorganic and hybrid lead-halide PQDs, we demonstrate a massive electro-switching effect observed via luminescence. The emission modulation is directly correlated with reduced photoluminescence lifetimes and can be attributed to a switching of radiative quantum efficiency. Furthermore, we present evidence for a memory effect that exhibits significantly delayed responses in comparison to the well-understood quasi-instantaneous Quantum-Confined Stark Effect that is also observable in these PQDs. In particular, the Stark effect is

utilized for the purpose of validating and comparing our measurements to those of conventional inorganic CdSe QDs, previously employed in ultrafast imaging of THz near-fields.

[1] M.B. Heindl, et al., Light Sci Appl 11, 5 (2022).

15 min. break

HL 45.5 Thu 16:15 POT/0006

Resolving Ultrafast Conductivity Dynamics in 2D-Perovskites via correlative THz-NIR Spectroscopy — •Lion Krüger[1], Fabian Brütting[1], Michael Baumann[2], Moritz B. Heindl[1], Maximilian Spies[3], Anna Köhler[3], Alexander JC Kühne[2], and Georg Herink[1] — [1]Experimental Physics VIII, University of Bayreuth, Germany — [2]Institute of Organic and Macromolecular Chemistry, Ulm University, Germany — [3]Experimental Physics II, University of Bayreuth, Germany

Quasi-2D Metal-Halide Perovskites offer flexible tuning of optoelectronic properties via composition and quantum confinement.

In this contribution we present measurements of the ultrafast carrier dynamics and mobilities of 3D- and quasi-2D-methylammonium lead iodide (MAPI) using optical-pump terahertz-probe spectroscopy (OPTP). The comparison with corresponding optical transient absorption measurements allows for the extraction of an ultrafast feature on a picosecond timescale that is correlated with the delayed hot-carrier cooling, known from 3D hybrid perovskites. Here this "hot phonon bottleneck" manifests as a 2D-specific, intensity-dependent signature in the THz-conductivity and is attributed to transient exciton formation [1].

[1] Lion Krüger, Fabian Brütting, Michael Baumann, Moritz B. Heindl, Maximilian Spies, Anna Köhler, Alexander JC Kühne, Georg Herink. "Confinement-induced Ultrafast Conductivity in 2D Perovskites resolved by correlative Terahertz-NIR Spectroscopy". 2025. In review.

HL 45.6 Thu 16:30 POT/0006

Intra- and Interlayer Excitonic Finestructure of $(PEA)_2PbI_4$ — •Patrick Grenzer[1], Fabian Lie[2], Klaus H. Eckstein[1], Linn Leppert[2], and Tobias Hertel[1] — [1]Institute of Physical and Theoretical Chemistry, Julius-Maximilians-University Würzburg, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Layered halide perovskites exhibit strongly bound excitons shaped by reduced dimensionality, dielectric confinement, and significant spinorbit coupling. Despite extensive work, the origin of the multiple resonances in absorption and PL of $(PEA)_2PbI_4$ remains subject to debate. We investigate the excitonic fine structure in high-quality, mechanically exfoliated single crystals by combining temperature- and polarization-resolved photoluminescence with first-principles GW+BSE calculations. The polarization dependence unambiguously assigns the observed features to distinct excitonic states and resolves the contributions from exchange interactions, crystal symmetry, and interlayer coupling. We further identify and spectroscopically separate intra- and interlayer excitons and their respective transition dipole moments. The results provide a consistent microscopic picture of the exciton manifold in $(PEA)_2PbI_4$ and clarify the origins of the multi-line structure characteristic of this material class.

HL 45.7 Thu 16:45 POT/0006

Dynamic Screening Effects on Auger Recombination in Metal-Halide Perovskites from First Principles — •Utkarsh Singh — Theoretical Physics Division, IFM, Linköping University, Sweden

Auger recombination is the dominant nonradiative loss in perovskite LEDs and nanolasers at carrier densities $> 10^{17}\,\mathrm{cm}^{-3}$.[1,2] Conventional first-principles treatments[3] use static dielectric screening $W(\mathbf{q}, 0)$ and neglect its frequency dependence in polar iodide perovskites.

I present a framework that incorporates the frequency-dependent screened interaction $W_{00}(\mathbf{q}, \omega)$, computed from low-scaling GW, into direct and phonon-assisted Auger amplitudes.[4] For γ-$CsPbI_3$ and γ-$CsSnI_3$, dynamic screening enhances the dielectric response at optical energies and reduces the room-temperature Auger coefficient by 50–60% compared with the static approximation.[5] The critical crossover density is shifted by a factor of 2, with implications for efficiency roll-off and lasing thresholds in optoelectronic devices.

These results establish dynamic screening as a quantitative determinant of Auger losses in polar semiconductors and provide a transferable framework for device modeling.

[1] J. Qin *et al.*, *Trends Chem.* **3** (2021). [2] Y. Sun *et al.*, *Appl. Phys. Rev.* **11** (2024). [3] E. Kioupakis *et al.*, *Phys. Rev. B* **92** (2015). [4] F. Yuan *et al.*, *Nat. Photonics* **18** (2024). [5] U. Singh & S. I. Simak, in preparation (2025).

HL 45.8 Thu 17:00 POT/0006

Influence of static disorder on the low temperature photoexcitation dynamics in triple cation lead halide perovskites — •Alexander Schauerte[1], Anton Krüger[1], Isabel Allegro[2], Dominik Muth[1], Ian Howard[2], Uli Lemmer[2], and Marina Gerhard[1] — [1]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Hans-Meerwein-Str. 4, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe, Germany

We study the recombination dynamics of phase stable triple cation lead halide perovskites $Cs_{0.1}(MA_{0.17}FA_{0.83})_{0.9}Pb_{1-x}(I_{0.84}Br_{0.16})_{3-2x}$ with intentionally induced deficiencies of Pb over a broad temperature range using time-resolved photoluminescence (PL) spectroscopy. In the temperature range below 70 K, we find pronounced sub-nanosecond PL dynamics which are accompanied by an increase of the carrier diffusivity by more than one order of magnitude. The findings are attributed to the polaronic Mott transition, beyond which polaron radii overlap, leading to efficient transport and bimolecular recombination. Moreover, the observed energy dependent PL dynamics at low temperatures indicate the presence of a phonon bottleneck, which inhibits efficient cooling of the excited population. We find that a higher degree of static disorder slows down bimolecular recombination, while the phonon bottleneck effect is more pronounced, potentially because slower recombination does not effectively reduce the hot carrier population.

HL 46: Ultra-fast Phenomena II

Time: Thursday 15:00–17:15 Location: POT/0051

HL 46.1 Thu 15:00 POT/0051

Ultrafast study of out-of-plane charge carrier diffusion in perovskite thin films via pump-probe sSNOM — •Daniel Sandner[1], Branden Esses[2], Zhao Yang[3], Kai Zhu[3], Joseph Berry[2,3], Hristo Iglev[1], and Markus Raschke[2] — [1]Laser- and X-ray physics E11, TU Munich — [2]CU Boulder — [3]NREL

Despite substantial evidence for polaron formation in lead halide perovskites (LHPs), which exhibit excellent photovoltaic performance, the role of polarons in transport remains unclear. We've measured diffusion with high spatial resolution by monitoring the carrier density at the top of a thin film via the tip-localized response in pump-probe mIR-sSNOM, while exciting the sample from below. Due to the small penetration depth of the pump beam, most electrons and holes are initially located at the bottom of the perovskite layer. Consistent with previous studies, we find local variations in the diffusion coefficient. To link transport and local structure, we employ a vibrational mode as an indicator of lattice stiffness and polaron formation [JACS 2024, 146(29), 19852-19862].

HL 46.2 Thu 15:15 POT/0051

Coherent exciton-phonon coupling and many body interactions in halide perovskites probed by 2D electronic spectroscopy. — •Mohsin Sayar[1], Katrin Winte[1], Davide Caratti[2], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Weizmann Institute of Science, Rehovot, Israel

Exciton-phonon interactions are central to the unique optoelectronic properties of halide perovskites. Here we use temperature-dependent two-dimensional electronic spectroscopy (2DES) with 10 fs time resolution to study the exciton dynamics in bulk $CH_3NH_3PbBr_3$ crystals. The 2DES maps distinguish between exciton and free-carrier-induced contributions to the near-band-edge optical nonlinearity, revealing distinct signatures of exciton-exciton and exciton-carrier many-body interactions. The ultrafast dynamics further reveal coherent low-frequency phonon oscillations at $40cm^{-1}$ and $67cm^{-1}$, corresponding to Pb-Br-Pb bending and stretching modes that most strongly couple to the exciton. Additionally, we observe faster, 105 fs exciton amplitude oscillations across all three crystal phases, arising from coherent population oscillations between 1s and 2p excitonic states, off-resonantly driven by the low-frequency coherent phonon fields in the crystal. We rationalize these results within a phenomenological model accounting for both exciton-phonon coupling and 1s-2p exciton coupling via the phonon fields. Preliminary polarization-resolved 2DES data show that these phonon-induced exciton oscillations are retained upon spin-selective excitation.

Invited Talk HL 46.3 Thu 15:30 POT/0051

Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes — Somayeh Souri[1], Katrin Winte[1], Daniel Lünemann[1], Daniel Timmer[1], Elena Mena-Osteritz[2], Sergei Tretiak[3], Christoph Lienau[1], and •Antonietta De Sio[1] — [1]Universität Oldenburg — [2]Universität Ulm — [3]Los Alamos National Laboratory

Non-equilibrium dynamics following photoexcitation in molecular materials arise from a complex interplay of electronic and vibrational motion, with antisymmetric vibrations playing a key role in ultrafast nonadiabatic dynamics, such as at conical intersections. Their direct spectroscopic identification is, however, challenging, since these modes are often Raman inactive and only weakly affect optical transitions. Here, we show experimental signatures of vibronic coupling to antisymmetric modes in the ultrafast symmetry-breaking dynamics of a quasi-quadrupolar dye[1,2] using two-dimensional electronic spectroscopy (2DES). The sub-50-fs 2DES maps reveal an asymmetric peak pattern with characteristic low-energy cross-peaks. We show that these peaks arise from stimulated emission from a double-minimum excited state potential energy surface induced by vibronic coupling to a ~1430 cm-1 antisymmetric mode[2]. Phenomenological essential state model simulations support the results. Our findings show that 2DES with sub-cycle vibrational resolution is a powerful method for identifying antisymmetric modes in the excited state dynamics prior to intramolecular vibrational relaxation and solvation. [1] Winte et al, Nature Chemistry 17, 1742 (2025); [2] Souri et al, submitted (2025)

15 min. break

HL 46.4 Thu 16:15 POT/0051

Investigating exciton dynamics and exciton–exciton interactions via optical two-dimensional photoelectron spectroscopy — •Luisa Brenneis[1], Matthias Hensen[1], Julian Lüttig[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Department of Physics, University of Ottawa, 150 Louis-Pasteur Pvt, Church St, Ontario K1N 6N5, Canada

Action-detected two-dimensional (2D) electronic spectroscopy has become a powerful technique to resolve exciton dynamics by measuring an incoherent signal proportional to the excited-state population generated by a multi-pulse sequence. However, processes that alter the excited-state population after the system's interaction with the pulse sequence, such as exciton–exciton annihilation, can obscure coupling signatures and single-exciton dynamics [1]. In optical 2D photoelectron spectroscopy (2DPES), typically a four-pulse sequence excites the system, followed by a time-delayed ionization pulse [2]. Here, we show how to disentangle exciton dynamics and interactions by varying the ionization pulse time delay. Exemplary simulations of a weakly coupled dimer demonstrate that short ionization delays reveal coupling signatures and single-exciton energy transfer, whereas longer delays reveal exciton–exciton annihilation. This concept is particularly promising for nanoscale surface studies, where 2DPES combined with photoemission electron microscopy enables spatially resolved exciton mapping.

[1] M. Bruschi et al., Phys. Chem. Lett. 14, 30, 6872 (2023).
[2] D. Uhl et al., Optica 8, 10, 1316 (2021).

HL 46.5 Thu 16:30 POT/0051

Ab initio Theory of Coherent Phonon Damping in Semimetals — •Yiming Pan and Fabio Caruso — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany

Coherent phonon plays an important role in the structural properties of the crystal lattice and ultrafast light-induced phase transition. Following its excitation, atoms oscillate coherently along the excited modes with decaying amplitudes. This dynamical process is commonly modeled with damping oscillators with phenomelogical damping rates. In this work, we derive this model by employing quantum kinetic equations [1], and attribute the damping rate and frequency renormalization of coherent phonon to the imaginary and real parts of the phonon self-energy. To valdiate our approach, we perform first-principles calculation of the damping rate of A_{1g} phonon arising from electron-phonon coupling and phonon-phonon coupling in semimetals Bi and Sb. The numerical results agree with available temperature- and fluence-dependent experimental data, thereby providing a predictive framework for determining the timescales of structural dynamics in driven solids.

[1] Y. Pan *et al.*, arXiv:2502.01529

HL 46.6 Thu 16:45 POT/0051

Probing Ultrafast Electronic and Lattice Dynamics simultaneously at the Atomic Scale with Time-Resolved Diffraction Anomalous Fine Structure (TR-DAFS) — •Moritz Meissner[1,2,6], T. C. Rossi[2], M. Rössle[2], C. Petersen[3], H. von Wenckstern[3], R. Mandal[4], M. Levantino[5], and R. M. van der Veen[2,6] — [1]Paul-Drude-Institut für Festkörperelektronik — [2]Helmholtz Zentrum Berlin — [3]Universität Leipzig — [4]Institut des materiaux de Nantes Jean Rouxel — [5]European Synchrotron Radiation Facility — [6]Technische Universität Berlin

This work presents the first successful demonstration of Time-Resolved Diffraction Anomalous Fine Structure (TR-DAFS) measurements carried out in a pump-probe (stroboscopic) scheme. We show that TR-DAFS can directly probe ultrafast structural and electronic dynamics in crystalline materials. Investigating Zinc oxide (ZnO) enables direct comparison between TR-DAFS at the Zn K-edge with time-resolved X-ray absorption spectroscopy (TR-XAS) data. TR-DAFS represents a leap forward in the study of photoexcited materials at the atomic scale by providing access to different aspects of lattice dynamics in resonant and non-resonant parts of the spectrum. Preliminary ab initio calculations show that the electronic changes visible in the resonant

part of the spectrum are associated with an increase of carrier temperature in the photoexcited state. This dual sensitivity to electronic and lattice degrees of freedom makes TR-DAFS a game-changer in investigating ultrafast processes in complex materials and heterostructures as represented by the results of this work.

HL 46.7 Thu 17:00 POT/0051

Theoretical Modeling of Ultrafast Phase Transitions from the Femtosecond to the Picosecond Scale — Stefano Mocatti, Giovanni Marini, Pierluigi Cudazzo, and •Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

In this talk, I will introduce a theoretical approach to ultrafast phase transitions that captures both electron/hole and phonon dynamics following laser pumping, on time scales ranging from a few femtoseconds to several picoseconds after irradiation.

At short times, the method relies on solving the Bloch equations coupled to Ehrenfest dynamics. It includes the electric field of the pump explicitly, as well as carrier-carrier, carrier-phonon, and phonon-phonon scattering, treated entirely from first principles.

At longer times before recombination, when carrier-carrier interactions generate a photoexcited quasi-equilibrium electron-hole plasma, the approach is based on a constrained density-functional perturbation theory (cDFPT) scheme that accounts for the presence of holes in the valence band and electrons in the conduction band (two-Fermi-level approach). In this framework, the calculation of forces, phonon dispersion, and carrier-phonon coupling becomes possible, as well as molecular dynamics with machine-learning potentials in the presence of an electron-hole plasma.

I will showcase applications of the method to several materials.

This work is funded by the European Union (ERC, DELIGHT, 101052708).

HL 47: 2D Materials VIII – Quantum emitters and defects

Time: Thursday 15:00–16:00 Location: POT/0081

HL 47.1 Thu 15:00 POT/0081

Tunable phonon sidebands of defect emitters in monolayer WSe_2 heterostructures — •Felix Schaumburg[1], Cornelius Diedrich[2], Alberto Rodriguez[2], Jeniffer König[2], Corinne Steiner[3], Patricia Pesch[3], Axel Lorke[1], Michael Lorke[1], Günther Prinz[1], Martin Geller[1], and Annika Kurzmann[2] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany — [2]II. Physikalisches Institut Fachgruppe Physik, Universität zu Köln, Germany — [3]Fachgruppe Physik, RWTH Aachen, Germany

Van der Waals heterostructures hosting single-photon emitters have emerged as a versatile platform for exploring material properties, like phonon interactions. We investigate single-photon emission from a heterostructure composed of a graphite back gate, hBN dielectric layers, and a monolayer of WSe_2. A 10 nm metallic top gate enables electrical tuning of the WSe_2 layer. The entire stack is strained using lithographically defined SiO_2 nanopillars. Optically active defect centers are introduced into the WSe_2 monolayer by electron-beam irradiation. These defect centers in the strained regions exhibit clear single-photon emission, confirmed by second-order correlation function values below 0.5. Voltage-dependent measurements reveal a pronounced Stark shift of the emission lines as well as electrically tunable phonon sidebands. The intensity evolution of these sidebands can be described within the framework of a Franck-Condon model. Our results demonstrate deterministic position control, electrical control, and phonon-sideband engineering of quantum emitters in WSe_2. This paves the way towards bright, electrically tunable emission in two-dimensional materials.

HL 47.2 Thu 15:15 POT/0081

Room Temperature Visualization of Exciton Confinement in Single Photon Emitters samples — •Lucas Liberal[1], Rafael Nadas[2], Frederico B. Sousa[1], Maria Clara Godinho[3], Gabriel Jacobsen[1], Takashi Taniguchi[4], Kenji Watanabe[4], Marcio Teodoro[1], Ado Jorio[3], and Leonardo Campos[3] — [1]Departamento de Física, Universidade Federal de São Carlos, São Carlos, Brasil — [2]Institut fur Physik, Humboldt-Universitat zu Berlin, Newtonstraße 15, Berlin, Germany — [3]Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brasil — [4]Research Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

Two-dimensional semiconductors such as monolayer WSe2 have attracted significant interest due to their remarkable quantum properties and their potential as scalable single-photon emitters. However, conventional micro-photoluminescence (μ-PL) techniques are fundamentally limited by optical diffraction, preventing direct access to critical nanoscale features such as strain gradients and highly localized quantum confinement. In this study, we employ tip-enhanced photoluminescence with a spatial resolution of 10 nm to image, at room temperature, the emission landscape of monolayer WSe2 suspended over nanopillars. Our measurements reveal two distinct localization regimes consistent with leading theoretical models for single-photon activation: one arising from intervalley defect exciton hybridization and another driven purely by strain-induced confinement. These results provide practical guidelines for the deterministic nanoengineering of quantum light sources.

HL 47.3 Thu 15:30 POT/0081

Beyond static defects: temporal evolution of defect-driven reliability in WSe2 — •Madhuri Chennur[1,2], Ulrich Kentsch[1], Jens Zscharschuch[1,2], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]TUD Dresden University of Technology, 01062 Dresden, Germany

Two-dimensional (2D) semiconductors are emerging as promising candidates for CMOS-compatible nanoscale electronics, where defects increasingly dictate electron transport. In WSe2 transistors, chalcogen vacancies commonly degrade hole mobility, yet defect-rich surfaces or interfacial contact layers have enabled ultra-low-barrier p-type contacts. However, the electrical role of these defects is almost exclusively interpreted through static pre- and post-irradiation comparisons, leaving the time-dependent evolution of engineered defect and irradiation-induced trap dynamics essentially unexplored.

Here, we present a weeks-to-months time-resolved optical-electrical study of WSe2 FETs irradiated with a single-dose broad-beam irradiation, followed by temporal tracking of threshold voltage, subthreshold swing, and hysteresis under constant bias and ambient conditions. Raman and PL spectroscopy performed in parallel reveal lattice disorder, oxidation, and adsorbate uptake. We observe a reproducible transition with shifts in electrical parameters, demonstrating that defect is intrinsically dynamic, not static. This coupled temporal mapping provides missing insight into defect-aware reliability for realistic ambient and radiation-relevant 2D electronics.

HL 47.4 Thu 15:45 POT/0081

Physical Drivers of Metal Adsorption at 2D Interfaces for Memristive Applications — •Manoj Dey[1], Hamid Mehdipour[1,2], Peter Kratzer[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin — [2]Faculty of Physics, University of Duisburg-Essen, Duisburg

Two-dimensional (2D) materials with engineered defects are emerging as promising candidates for next-generation memristors. In these "atomristors," resistive switching (RS) arises from atomic-scale processes at the electrode-2D interface. Experiments show that adsorption and desorption of electrode metal atoms at vacancies play a key role in RS [1]. Here, we combine hybrid density functional theory with many-body dispersion corrections and the Sure Independence Screening and Sparsifying Operator (SISSO) method [2] to study metal adsorption on transition-metal dichalcogenides at gold interfaces. SISSO provides a predictive model for adsorption energies and uncovers the fundamental physical factors driving RS. Our sensitivity analysis shows how orbital hybridization and bonding interactions dominate the behavior, offering simple heuristics for understanding the atomic processes. We also build a materials-property map that highlights promising candidates and connects our predictions with experimentally demonstrated devices. Together, these results link fundamental material descriptors to RS behavior and offer clear guidance for designing future 2D atomristors.

[1] Ruijing Ge *et al.*, *Adv. Mater.*, **33**, 2007792 (2021).
[2] R. Ouyang *et al.*, *Phys. Rev. Materials*, **16**, 2, 083802 (2018).

HL 48: Heterostructures, Interfaces and Surfaces: Fabrication and Structure

Time: Thursday 15:00–17:15 Location: POT/0251

HL 48.1 Thu 15:00 POT/0251

Cross-sectional scanning tunneling microscopy (XSTM) study of nearly lattice-matched III-V semiconductor heterostructures — •Hitesh Kumar[1], Rüdiger Schott[2], Zijin Lei[2], Werner Wegscheider[2], and Stefan Fölsch[1] — [1]Paul Drude Institute for Solid State Electronics, Berlin, Germany — [2]Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland

XSTM is a powerful technique for investigating the structural and electronic properties of III-V semiconductor heterostructures. These heterostructures are grown along the [001] direction by molecular beam epitaxy and accessible in cross-sectional view by cleaving the sample in ultrahigh vacuum to expose the (110) cleavage surface. We used this approach to study a GaSb-InAs-AlGaSb-InAs-InAsSb layered heterostructure grown on a Te-doped GaSb substrate. Voltage-dependent chemical contrast in STM imaging allows differentiation between anions and cations in the III-V semiconductors. Using this capability, we analyzed the degree of homogeneity in the ternary materials (Al-Ga mixing in the AlGaSb layer and As-Sb mixing in the InAsSb layer). With the help of scanning tunneling spectroscopy, we precisely determined the band gaps of the individual layers and locally probed the band lineup across the entire heterostructure. This allowed us to investigate the behavior of charge carriers governed by the band lineup. Specifically, we studied the spatial confinement and quantization of conduction band states in the InAs layer and their decay into the gap region of the adjacent layers.

HL 48.2 Thu 15:15 POT/0251

Theoretical Exploration of the Electronic Structure at Group-III Nitride Interfaces — •Maximilian Lauer[1,2], 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]Zentrum für Materialforschung (ZfM), Justus-Liebig-Universität Gießen, Germany

Group-III nitrides are an essential group of materials at the forefront of modern optoelectronics. Recently, the metastable zincblende (In,Ga)N system emerged as a promising material for optoelectronic devices. Heterojunctions play a central role in device design, making a precise understanding of their electronic structure essential. Determining the band alignment at the interface is crucial for understanding its electronic properties.

Here, we show that the zb-GaN/zb-InN heterojunction exhibits a Type-I alignment with no states forming within the band gap at the interface. We performed KKR calculations with LDA-1/2 band gap corrections on coherently strained supercells. We report values for the band offset parameters and explore the microscopic electronic structure at the interface. Our calculations demonstrate the importance of band corrections for calculating electronic structure parameters, such as band offsets, and provide a basis for further investigations into the (Ga,In)N alloy system using the CPA.

HL 48.3 Thu 15:30 POT/0251

GaPN growth on As-Modified Si(100) for defect-reduced heteroepitaxy — •Hitha Haridas[1], Kai Daniel Hanke[1], Agnieszka Paszuk[1,2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau,Germany — [2]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany

The Monolithic integration of III-V semiconductors with Si(100) offers a promising route toward high-efficiency,low-cost optoelectronic devices. Among these materials, GaPN is a promising candidate for III-V/Si integration because it can be grown lattice-matched to silicon, thereby minimizing strain and reducing the formation of misfit dislocations. However, structural defects generated during the earliest stages of growth can propagate into subsequent epitaxial layers, ultimately limiting device performance. In this study, we investigate the nucleation and early-stage growth behavior of GaPN on As-modified Si(100) surfaces by combining ex situ surface morphology analysis,electron channeling contrast imaging, and in situ optical spectroscopy.This integrated approach allows us to systematically evaluate how variations in the initial growth conditions influence defect formation. The insights gained provide broader guidance for improving interface quality and advancing III-V/Si heteroepitaxy through more precise control over the initial growth phases.

HL 48.4 Thu 15:45 POT/0251

Acoustoelectric effect in organic-inorganic semiconductor systems — •Paromita Bhattacharjee[1], Patrick Ganswindt[2], Alexander S. Urban[2], and Hubert Krenner[1] — [1]Institute of Physics, University of Münster, Germany — [2]Faculty of Physics, Ludwig-Maximilians-Universität München, Germany

Surface acoustic waves (SAWs) are elastic waves propagating on the surface of a piezoelectric solid and while interacting with a semiconductor, its strain and piezoelectric fields modulate the band-gap. Strain-induced field imposes an acoustoelectric (AE) drag on the charges in the direction of SAW propaga-tion, and in a photoconductive semiconductor, excitons get ionized by piezoelectric field into separate elec-trons and holes, captured and transported by SAW [1]. Utilizing these effects, we present first study of SAW-induced charge transport in hybrid organic-inorganic semiconductor system of organic polymer, poly(3-hexylthiophene) (P3HT) and halide perovskite (CsPbBr3 and CsPb(IxBr1-x)3) nanowires (HPNWs). In samples with only HPNWs the total AE current nearly vanishes due to comparable electron-hole mobilities in these materials [2]. However, in hybrid layers, weak AE effect is observed with CsPb(IxBr1-x)3 NWs and a hole dominated AE transport with CsPbBr3 NWs. The band realignment at the heterojunction explains that while for CsPb(IxBr1-x)3 -P3HT ambipolar electron-hole transport occurs via the NWs, for CsPbBr3-P3HT, electrons are limited by low electron mobility in P3HT. References: [1] J. Phys. D: Appl. Phys. 57, 423001 (2024). [2] Nano Lett., 19, 8701-8707 (2019).

15 min. break

HL 48.5 Thu 16:15 POT/0251

Ultra-high vacuum exfoliation method for the preparation of large-area single layer TMDC films — •Zhiying Dan[1], Ronak Sarmasti Emami[1], Antonija Antonija Grubisic-Cabo[1], Petra Rudolf[1], Deepnarayan Biswas[2], and Tien-Lin Lee[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands — [2]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK

Two-dimensional transition metal dichalcogenides (2D TMDCs) are promising candidates for next-generation electronic, optical, and spintronic devices. While mechanical exfoliation yields high-quality 2D flakes, their lateral size is typically limited to tens of micrometers. Here, we report the preparation of 2D WS2 and WSe2 using a recently developed kinetic in situ single-layer synthesis (KISS) method, performed in ultra-high vacuum and tailored for surface science studies. We examine how substrate choice and chalcogen species affect film size and quality using X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy, and X-ray standing waves (XSW). Our results show that the quality of the bulk TMDC crystal is crucial for successful KISS exfoliation. Moreover, preliminary XSW data suggest that KISS does not degrade the underlying substrate, highlighting its potential as a non-destructive approach for 2D material synthesis.

HL 48.6 Thu 16:30 POT/0251

Electrical conduction and sensing properties of contacted CNTs after MOF synthesis — •Marvin J. Dzinnik[1], Adrian Hannebauer[2], Feriel Friha[1], Andreas Schaate[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hanover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hanover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hanover, Germany

Metal-organic frameworks (MOFs) are a versatile sensor material: they are tunable, highly porous, and can be precisely grown on carbon nanotubes (CNTs).[1]

Here, we investigate how UiO-66 MOF growth affects single nanotubes. We performed DC measurements on contacted multi-walled carbon nanotubes (MWCNTs) before and after UiO-66 synthesis. We observe pronounced changes in both magnitude and character of the electrical response, indicating a strong interaction between MWCNT

and MOF. AC measurements show a linear response to ethanol vapor up to 40 000 ppm, suggesting that single MWCNT-MOF hybrids are promising, tunable gas-sensing elements.

[1] Dzinnik, M. J. et al. Commun Mater 5, 38 (2024).

HL 48.7 Thu 16:45 POT/0251

Nucleation behavior for remote epitaxy of GaAs and AlAs on carbon-covered GaAs substrates — •Binamra Shrestha, Tobias Henksmeier, and Dirk Reuter — Paderborn University, Paderborn, Germany

Recently, remote epitaxy was proposed as a method that enables the growth of free-standing single-crystal layers and substrate reuse by using atomically thin 2D materials as release layers. In this work, we investigate the epitaxial growth behavior of GaAs and AlAs on ultrathin amorphous carbon layers deposited by PECVD on GaAs substrates. The amorphous carbon exhibits a graphene-like structure consisting predominantly of in-plane sp^2 bonding, thereby serving as a quasi-2D template capable of transmitting the substrate's electrostatic potential for remote epitaxial growth.

We performed controlled nucleation studies using molecular beam epitaxy (MBE). First, a GaAs buffer layer is grown on the bare GaAs to planarize the substrate surface, then the sample is covered with amorphous carbon. Subsequently, ultrathin GaAs layers ranging from 0.25 nm to 2 nm are deposited on the graphene/GaAs template at 300 °C, and the resulting nuclei are examined via atomic force microscopy (AFM). Nucleation is first observed at approximately 0.37 nm deposition thickness, with nuclei predominantly aligned along atomic steps. This strong step-edge preference indicates that remote epitaxy is the dominant mechanism, compared to pinhole-initiated nucleation. These results highlight the suitability of PECVD-deposited amorphous carbon as an effective 2D interlayer for remote epitaxy.

HL 48.8 Thu 17:00 POT/0251

Quantum confinement in semiconductor random alloys: a case study on Si/SiGe/Si — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

When the size of random alloys is reduced, local fluctuations of alloy composition become more influential. Using extended Hückel theory, we study the semiconductor alloy SiGe sandwiched between Si due to its relevance in semiconductor devices. We evaluate the effects of the alloy composition, layer thickness, and local fluctuations of the Ge concentration on band alignment and the band gap. Results are compared to the finite quantum well model. This model captures the essenial physics and can act as a computationally faster surrogate model.

HL 49: Quantum Emitters in 2D Semiconductors

Time: Thursday 16:15–17:30 Location: POT/0081

Invited Talk HL 49.1 Thu 16:15 POT/0081

Phonon-mediated nonlinearity and defects in hexagonal boron nitride — •Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Germany

Hexagonal boron nitride (hBN) hosts a rich phonon landscape whose strong oscillator strengths in the first and second Reststrahlen bands give rise to negative permittivity and support the propagation of hyperbolic phonon polaritons. In this work, we show that these phonon modes can mediate highly efficient down-conversion of optical excitation, enabling strong coupling to point defects and facilitating the coherent excitation of their electronic states. We further demonstrate that such defect states in hBN can couple efficiently to excitons in hybrid hBN*perovskite structures, establishing a robust exciton*defect interaction channel. Remarkably, we find that excitonic energy can be transported over distances up to 150 micrometers through incoherent hopping across a defect network within hBN. By combining spatially and spectrally resolved photoluminescence and cathodoluminescence spectroscopy, we identify the mechanisms governing coherent and incoherent defect excitation and reveal the interplay and strong coupling among excitons, defects, and phonons in hBN. These insights establish hBN as a versatile platform for phonon-assisted light*matter interactions and long-range energy transport in hybrid quantum nanophotonic systems.

HL 49.2 Thu 16:45 POT/0081

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-Universität 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 spin triplet system of the lately discovered negatively charged boron vacancy ($V_B{}^-$) in hexagonal boron nitride (hBN) can be exploited in terms of its application as temperature, magnetic field, and pressure sensor.[1] Increasing the sensitivity of these nano-scale sensors is a crucial step towards application and requires not only controlled generation[2] but deep knowledge about the dynamics of the system. This includes predicted but experimentally hardly accessible intermediate states.

In this study, we achieve a direct measurement of a 24.0(3) ns relaxation time from the dark intermediate state to the ground state at room temperature, which approximately doubles at low temperatures. These findings are corroborated by detailed simulations of populations. Accounting for this relaxation considerably enhances spin manipulation efficiency, allowing substantial optimization of the quantum sensor's sensitivity based on boron vacancies.[3]

[1] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).
[2] Patra et al., *Adv. Funct. Mater.* e17851 (2025).
[3] Konrad et al., *arXiv* preprint arXiv:2503.22815 (2025).

HL 49.3 Thu 17:00 POT/0081

Exciton-enhanced light emission in pristine and doped MoS_2 from ab initio calculations — •Adriana Bocchini[1], Djennane Khaoula[2], Henry Hübschmann[1], Nikita Siverin[3], Andreas Farenbruch[3], Maja Groll[1], Klaus Jöns[1], Gerhard Berth[1], Dmitri Yakovlev[3], Wolf Gero Schmidt[1], and Uwe Gerstmann[1] — [1]Universität Paderborn, Germany — [2]Yahia Fares University of Medea, Algeria — [3]Technische Universität Dortmund, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) are emerging as a suitable alternative in a variety of electronic and optoelectronic devices [1,2]. The properties of this family, in fact, can be systematically customized upon structural modification, e.g., via exfoliation or dopants. Notably, most of these properties are strongly determined by excitons, the formation of which is strongly facilitated by defects [3]. In this study, we use DFT routines to systematically investigate the influence of excitons on the optical properties of MoS_2 films. Thereby, we do not only analyze the dependency of the optical response on the layer thickness, but also their evolution upon the application of external electric fields or by twisting the layers relative to each other. In addition, we model MoS_2-based Janus structures by selectively substituting some of the S atoms with heavier chalcogens and analyze the suitability of these configurations as possible light-emitting solid-state quantum dots.

[1] R. Thayil,, *et al.*, Small **21**, 2412467 (2025)
[2] S. Joseph, *et al.*, Mater. Chem. Phys. **297**, 127332 (2023)
[3] J. Qu *et al.*, ACS Nano **18**, 34322 (2024)

HL 49.4 Thu 17:15 POT/0081

Thermodynamic properties of quantum defects in boron nitride using machine-learned force fields — •Ariel Moises Cabrera Aguilar and Carla Verdi — The University of Queensland, Brisbane, Australia

Hexagonal boron nitride (hBN) has emerged as an excellent host material for bright single-photon emitters. Experimental and computational studies associate these single-photon emitters (SPEs) in hBN predominantly with carbon-related defects. However, the lack of first-principles calculations at finite temperatures and with sufficiently large supercells hinders the establishment of a consensus on the most likely defect can-

didates for quantum-technology applications. Machine-learned force fields (MLFFs) provide highly accurate finite-temperature simulations because they can be trained to reproduce first-principles energies and forces across diverse configurations. We trained a MLFF capable of describing various carbon cluster defects (C_B, C_N, C_BC_N, C_BV_N, C_BC_i, and C_NC_i) at temperatures up to approximately 2000 K. To evaluate the accuracy of the force field in reproducing atomic positions, interatomic energies, and forces across these structures, we compute formation energies, phonon dispersions, and photoluminescence spectra, and compare these quantities with available experimental data. The force field successfully reproduces the line shape of several defects in multilayered systems of different supercell sizes. The MLFF is used to investigate multiple defects in large supercells over long molecular dynamics simulation times, allowing us to capture metastable structures that emerge at finite temperature.

HL 50: Members' Assembly

Organized by Rudolf Bratschitsch, Alexander Holleitner and Axel Lorke

Time: Thursday 17:45–19:15 Location: POT/0051

All members of the Semiconductor Physics Division are invited to participate.

HL 51: 2D Materials: Stacking and heterostructures (joint session O/HL/TT)

Time: Friday 9:30–12:30 Location: HSZ/0401

HL 51.1 Fri 9:30 HSZ/0401

A new fabrication method for metal intercalated epitaxial graphene devices — •Marc Bothe[1], Stefan Wundrack[1,2], Marcelo Jaime[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Hans Werner Schumacher[1], Andrey Bakin[2], and Teresa Tschirner[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany

Epitaxial graphene grown on silicon carbide is a promising platform to achieve metal intercalation. It enables the creation of two-dimensional metal layers that are encapsulated and protected by graphene. However, the use of metal intercalated graphene samples for lithographic device fabrication presents two critical challenges. First, solvents used in the lithography process lead to the deintercalation of the metal atoms. Second, the presence of lattice defects in the graphene - necessary for the intercalation process - compromises the structural and electronic integrity of the device. We present a novel fabrication method that solves these problems. In our approach, the graphene devices are first pre-structured using lithography and subsequently intercalated. This is made possible by a spatial separation on the sample between the device structures and the intercalation origin and by intercalation channels that can guide the intercalation front reliably to the devices. We demonstrate this method on gallium intercalated epitaxial graphene Hall bars that exhibit superconducting behaviour.

HL 51.2 Fri 9:45 HSZ/0401

Anisotropic Strain Observation in Naturally Occurring Buckling on Twisted Bilayer Graphene: A Nano-Raman Study — •Gustavo Soares[1], Rafael R. Barreto[1], Rafael Nadas[1], Kenji Watanabe[2], Takashi Taniguchi[2], Leonardo C. Campos[1], Luiz G. Cancado[1], and Angelo Malachias[1] — [1]Physics Department, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, 31270-901, Brazil — [2]National Institute for Materials Science, Tsukuba, Ibaraki, 3050047, Japan

This work investigates naturally occurring buckling and its relation with anisotropic strain relaxation in twisted bilayer graphene (tBG). In the tBG system a twist angle is imposed to influence graphene structural and electronic properties. Such condition directly implies in the occurrence of biaxial in-plane strain, with usual observation of buckled/wrinkled localized regions where the tBG morphology is no longer planar. Using tip-enhanced Raman spectroscopy, we conducted high-resolution mapping to analyze variations in Raman bands associated with twist angle variation and strain effects. Our findings reveal that localized strain gradients, modulated by twist angle variations, induce deterministic buckling in graphene layers, evidencing distinct uniaxial and biaxial strain regions. Finite element modeling further supports these observations, showing that buckling can store elastic energy sufficient to overcome usual tBG-substrate adhesion forces.

HL 51.3 Fri 10:00 HSZ/0401

Kirkendall Voids in Monolayer $Mo_xTa_yS_2$ Alloys on Au(111) — Kai Mehlich[1], Thais Chagas[1], Francis H. Davies[2,3], Alessia Bardazzi[1], Catherine Grover[1], Arkady V. Krasheninnikov[3], and •Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen, Germany — [2]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter, EX4 4QL United Kingdom

During the growth of monolayer MoS_2-TaS_2 heterostructures, we observe the Kirkendall effect: Diffusing vacancies agglomerate in MoS_2, forming what are commonly termed Kirkendall voids - here manifesting as holes in the 2D layer. This phenomenon has not been previously reported in systems with reduced dimensionality.

We prepare the lateral heterostructures by reactive molecular beam epitaxy on chemically inert and weakly interacting Au(111). First, compact MoS_2 cores are grown. In a second step, TaS_2 is added in a sulfur-rich environment at elevated temperatures which promotes diffusion at the interface. The resulting heterostructures exhibit characteristic 2D Kirkendall holes surrounded by a $Mo_xTa_yS_2$ alloy region. These findings reveal defect-mediated processes in low-dimensional systems and open new avenues for designing 2D lateral heterostructures with intricate morphologies.

HL 51.4 Fri 10:15 HSZ/0401

Designing 2D Non-van der Waals Heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Heterostructure interfaces created by stacking two-dimensional (2D) materials offer a pathway to realizing advanced electronic and magnetic functionalities at the nanoscale. In this work, we present a high-throughput screening of non-van der Waals (non-vdW) 2D heterostructures; including sandwich-like stacking. Non-van der Waals 2D materials can be obtained by both top-down exfoliation as well as bottom-up growth approaches of non-layered bulk crystals [1]. Our approach uses the AFLOW-Hetbuilder - a newly developed tool for stacking 2D systems based on the coincidence lattice algorithm [2-4].

We investigate interfacial binding effects across a wide range of heterobilayers [5] and sandwich-like systems, analyzing their structural, electronic, and magnetic characteristics such as hybrid interface bands and robust magnetic coupling. Furthermore, we compare the binding energetics of non-vdW and conventional vdW heterostructures. The tunable interfacial properties of non-vdW 2D heterostructures provide a versatile platform for advanced functionalities with potential applications in electronics, spintronics, and the energy sector [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989, (2022).
[2] D.S. Koda *et al.*, J. Phys. Chem. C **120**, 10895, (2016).
[3] https://zenodo.org/record/4721346 .
[4] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[5] A. Nihei, *et al.*, arXiv DOI: 10.48550/arXiv.2503.12209 (2025).

HL 51.5 Fri 10:30 HSZ/0401

Second-Order Nonlinear Imaging for Probing 2D van der Waals Structures — •Tao Yang[1], Ben John[1], Kyoung P. Lee[2], Nasim Mirzajani[1], Martin Wolf[1], Xiaoqin Li[2], Martin

Thaemer[1], Alexandar Paarmann[1], Niclas S. Mueller[3], and Alexander P. Fellows[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas at Austin, Austin, USA — [3]Freie Universitaet Berlin, Berlin, Germany

Twisted and stacked multi-layer architectures offer new opportunities for tailoring the electronic and optical properties of two-dimensional (2D) van der Waals materials. Reliable determination of crystal structure, stacking sequence, and twist angle is therefore crucial. Second-order nonlinear optical microscopy, including second-harmonic and sum-frequency generation (SHG and SFG, respectively), provides high sensitivity to crystal symmetry and orientation in non-centrosymmetric lattices. Recently, we employed heterodyne-detected vibrational SFG microscopy to probe the local structure of hexagonal Boron Nitride (hBN) monolayers with sub-micron resolution. By employing our developed azimuthal-scanning approach, we fully resolved the crystallographic structure and edge termination in monolayer flakes. Here, we extend these measurements to multi-layer hBN structures, using the same azimuthal-scanning approach in a newly developed SHG microscope to gain insight into their different stacking configurations. Our results highlight second-order nonlinear microscopy as a powerful tool for quantitative structural analysis in 2D materials and for future studies of moiré and twisted heterostructures.

HL 51.6 Fri 10:45 HSZ/0401

Moiré-Driven Electronic Modulations in Weakly Coupled h-BN/Graphite — •Fábio J. R. Costa[1,2,7], Daniel Arribas[2], Thiago G. L. Brito[2], Tin S. Cheng[3], Jonathan Bradford[3], Amelia Thompson[3], Alex Saywell[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergey V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Luiz F. Zagonel[1], Klaus Kuhnke[2], Klaus Kern[2,6], and Anna Rosławska[2] — [1]University of Campinas, Brazil — [2]Max-Planck-Institut für Festkörperforschung, Germany — [3]University of Nottingham, UK — [4]Laboratoire Charles Coulomb, France — [5]Institut Universitaire de France, France — [6]EPFL, Lausanne, Switzerland — [7]Current address: Université de Strasbourg, CNRS, IPCMS, Strasbourg, France

Van der Waals materials and their heterostructures offer exciting opportunities for next-generation nanophotonic and electronic technologies. Their electronic and optical properties can be modulated by moiré superlattices that emerge when mismatched layers are stacked together. Hexagonal boron nitride (h-BN) is a key platform in this context, yet the influence of moiré patterns on weakly interacting h-BN interfaces remains underexplored. Here[1], we use scanning tunneling microscopy to resolve large moiré superlattices in h-BN/graphite and uncover pronounced nanoscale modulations of the electronic landscape, despite their weak interlayer interactions. These findings position moiré engineering in h-BN as a powerful tool to tailor local functionalities in van der Waals heterostructures. Ref.: 1. Fábio J. R. Costa *et al.* ACS Nano 2025 19 (40), 35528-35538

HL 51.7 Fri 11:00 HSZ/0401

μ-ARPES study on the fine electronic structure of misfit layer compound (PbSe)1.16(TiSe2)2 — •Haruki Muramatsu[1], Natsuki Mitsuishi[2,3], Teppei Ueno[4], Kenichi Ozawa[5], Kaya Kobayashi[4,6], and Kyoko Ishizaka[1,2] — [1]Dept. of Appl. Phys. & QPEC, Univ. of Tokyo — [2]CEMS, RIKEN — [3]Grad. Sch. Sci., Nagoya Univ. — [4]Dept. of Physics, Okayama Univ. — [5]KEK-PF — [6]RIES, Hokkaido Univ.

Misfit layered compounds have been attracting significant attention due to their lattice mismatches and resultant two-dimensional electronic structures reminiscent of van der Waals heterostructures. One such compound, (PbSe)1.16(TiSe2)2, consists of alternating stacking of PbSe monolayers (NaCl-type, four-fold symmetry) and TiSe2 bilayers (CdI2-type, three-fold symmetry). To elucidate its electronic structure, we performed μ-ARPES measurements by carefully distinguishing the cleavage surface terminations. In the presentation, we will discuss the novel electronic states reflecting the natural incommensurate heterostructure as well as charge density wave in the buried TiSe2 bilayer.

HL 51.8 Fri 11:15 HSZ/0401

Twisted $NbSe_2$ heterostructures — •Alexander Bäder[1,2], Clara Pfister[3,4], Tobias Wichmann[1,5], Laura Pätzold[3,4], Tim O. Wehling[3,4], and Felix Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]I. Institute of Theoretical Physics, U Hamburg — [4]The Hamburg Centre for Ultrafast Imaging — [5]Institut für Experimentalphysik IV A, RWTH Aachen

We fabricated monolayers (MLs) of the van der Waals material $NbSe_2$ that are rotated with respect to the underlying bulk $NbSe_2$ using our developed ultra-high vacuum (UHV) stacking technique. These heterostructures were characterized through the use of scanning tunneling microscopy and spectroscopy at a base temperature of 1.4 K. The MLs realize a variety of twist angles relative to the underlying bulk lattice, with the lowest observed twist angle being 10°. The MLs display the coexistence of charge density waves (CDW) and moiré effects: In the absence of strain, the MLs develop a 3×3 CDW, however the application of strain through interfacial disorder results in a 2×2 CDW state, supported by theoretical calculations. Compared to isolated MLs the superconducting order parameter is enhanced due to the proximity effect from the underlying bulk.

HL 51.9 Fri 11:30 HSZ/0401

band structure and charge density wave in a natural van der Waals heterostructure 4Hb-TaSe2 — •Fumihiko Kimura[1], Tomoki Maeda[2], Natsuki Mitsuishi[3,4], Kazuki Okada[2], Takuya Nomoto[5], Kenichi Ozawa[6], Masahiro Naritsuka[3], Tetsuo Hanaguri[3], Shunsuke Kitou[7], Yuiga Nakamura[8], Taka-hisa Arima[3,7], Takao Sasagawa[2], and Kyoko Ishizaka[1,3] — [1]Quantum-Phase Electronics Center & Department of Applied Physics, The University of Tokyo — [2]Laboratory for Materials and Structures, Science Tokyo — [3]RIKEN CEMS — [4]Graduate School of Science, Nagoya University — [5]Department of Physics, Tokyo Metropolitan University — [6]Institute of Materials Structure Science, High energy Accelerator Research Organization (KEK) — [7]Department of Advanced Materials Science, The University of Tokyo — [8]Japan Synchrotron Radiation Research Institute (JASRI), SPring-8

4Hb-TaSe2 is a natural van der Waals heterostructure charge density wave (CDW) material consisting of alternative stacking of monolayer 1T-TaSe2 (Mott insulator with Star-of-David CDW) and monolayer 2H-TaSe2 (superconductor with 3 by 3 CDW). Although transport measurements have suggested the existence of multiple CDWs, the details of the CDW and electronic structures remain unclear. In this study, we directly observed the electronic structure of 4Hb-TaSe2 by micro-focused angle-resolved photoemission spectroscopy with careful selection of the surface terminations. We discuss the temperature dependent electronic structure with comparison to the CDW structures obtained by scanning tunneling microscopy and X-ray diffraction.

HL 51.10 Fri 11:45 HSZ/0401

Coexisting charge density waves in twisted NbSe2 bilayers — •Christopher Tat Shun Cheung[1], Zachary A. H. Goodwin[2], Yixuan Han[3], Jiong Lu[3], Arash A. Mostofi[1], and Johannes Lischner[1] — [1]Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K. — [2]Institute for Functional Intelligent Materials, National University of Singapore, Singapore 117544, Singapore — [3]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Twisted bilayers of semiconducting transition metal dichalcogenide (TMD) monolayers have been studied extensively. In contrast, twisted bilayers composed of metallic monolayers, such as NbSe2, remain less understood.

Monolayer NbSe2 can host different types of charge density waves (CDWs), in which the Nb atoms move away from their high-symmetry positions. In twisted bilayer NbSe2, identifying CDWs in relaxed structures is challenging because atomic relaxations occur both because of CDW formation and also because of the moiré pattern.

We have carried out large-scale first-principles calculations using density functional theory to study the moiré relaxations and CDWs in twisted bilayer NbSe2. We have developed methods for revealing the CDWs, and for locally classifying the type of CDW. We find that different types of CDWs coexist in the moiré unit cell due to the interactions with strain induced by moiré relaxations [1].

[1] Cheung et al, Nano Lett. 2024, 24, 12088-12094.

HL 51.11 Fri 12:00 HSZ/0401

MicroARPES studies of contact doping of monolayer transition metal dichalcogenides by RuCl3 — •Thomas Nielsen[1], Edvard Solbrekken[1], Alfred J. H. Jones[1], Zhihao Zhiang[1], Chakradar Sahoo[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jill A. Miwa[1], Søren Ulstrup[1], Christian Overby[1], and Christian V-B. Fokdal[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan

Placing van der Waals materials into contact with α-$RuCl_3$ has recently emerged as a method of modulating their electronic structures. The proximity to α-$RuCl_3$ has been observed to produce strong hole doping in the van der Waals material, and this has been established as a method to create better electrical contacts in transistor devices based on monolayer transition metal dichalcogenides (TMDs). Here, we use the microARPES endstation at the ASTRID2 synchrotron light source at Aarhus University in Denmark to study the valence bands and core levels of semiconducting monolayer TMDs in proximity to α-$RuCl_3$. We observe a large valence-band shift of $0.7-0.8$eV indicating strong hole doping. α-$RuCl_3$ is highly sensitive to the temperatures and chemicals typically used in the dry-transfer fabrication procedures of van der Waals heterostructures. How the degradation of α-$RuCl_3$ affects the proximity-induced doping of the TMD is discussed based on the ARPES measurements.

HL 51.12 Fri 12:15 HSZ/0401

STEM Investigation of Entropy Forbidden Ordering in CVD Grown WSe_2-$MoSe_2$ Alloys — •Max Bergmann[1], Matvei Kislitsyn[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

2D transition metal dichalcogenides have gained significant interest due to their optoelectronic properties, which can be tailored by structural variation. However, controllable production, namely growth, of such tailored structures still remains a key challenge towards large-scale production. In this study, we show lateral heterostructures of 2D $MoSe_2$ and WSe_2, grown on a SiO_2 TEM grid by chemical vapor deposition, that at the interface show a highly ordered structure of W and Mo atoms at the TMD positions, as observed by scanning transmission electron microscopy. This is in contrast to *ab initio* calculations, which ascribe unordered alloys as the preferred configuration, since entropy is the main driving force compared to formation enthalpy. We link this unexpected phenomenon to the initial nucleation of the material on a clean $MoSe_2$ crystal edge, present before the alloy growth, together with special precursor chemistry. Furthermore, we show *ab initio* results in conjunction with the special quasirandom structure method on the bandstructure and optical properties of this structure.

HL 52: THz and MIR Physics in Semiconductors

Time: Friday 9:30–10:45 Location: POT/0006

HL 52.1 Fri 9:30 POT/0006

Probing Terahertz Emission and Structural Dynamics in Quasi-two-dimensional $NbOI_2$ — •Daniel Geyer[1], Rieke von Seggern[1], Soufiane El-Kabil[1], Zouchen Fu[3], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Germany — [3]Nankai University, Tianjin, China

Optically induced processes in matter, captured via time-resolved imaging methodologies, uncover a variety of transient phenomena evolving on ultrafast time scales. Layered ferroelectric niobium oxide dihalides $NbOX_2$ (X=I, Cl, Br) have garnered significant interest in this context, as they combine pronounced optical nonlinearities [1,2] with a ferroelectric order parameter that can be controlled via optical stimuli [3]. In this work, we investigate the $NbOI_2$ compound as a material platform in which both regimes of ultrafast light-matter interaction can be accessed within different experimental approaches.

At first, we explore thin $NbOI_2$ flakes as promising stackable terahertz (THz) emitters. We demonstrate broadband THz generation via nonlinear optical rectification, characterized using a time-domain THz emission spectroscopy setup.

Secondly, we discuss the photoinduced evolution of the material's ferroelectric polarization, employing time-resolved electron diffraction in an ultrafast transmission electron microscope (UTEM).

[1] Guo et. al., Nature **613**, 53-59 (2023)
[2] Chen et. al., Adv. Mater. **36**, 2400858 (2024)
[3] Wang et. al., Nat. Comm. **16**, 8132 (2025)

HL 52.2 Fri 9:45 POT/0006

AlGaN/GaN-based grating-gate plasmonic crystals for nonlinear THz applications — Pavlo Sai[1], Vadym V. Korotyeyev[2], Serhii Kukhtaruk[2], Dmytro B. But[1], Maksym Dub[1], Alexej Pashkin[3], Stephan Winnerl[3], Wojciech Knap[1], and •Martin Mittendorff[4] — [1]Institute of High Pressure Physics PAS ul. Sokołowska 29/37, Warsaw 01-142, Poland — [2]V. Ye. Lashkaryov Institute of Semiconductor Physics (ISP) NASU prospect Nauky 41, Kyiv 03028, Ukraine — [3]Helmholtz-Zentrum Dresden-Rossendorf 01328 Dresden, Germany — [4]Universität Duisburg-Essen Fakultät für Physik 47057 Duisburg, Germany

We present time-resolved THz measurements on grating-gate plasmonic crystals, based on the two-dimensional interface electron gas in epitaxial GaN/AlGaN heterostructures. The free-electron laser FELBE at Helmholtz-Zentrum Dresden-Rossendorf served as tunable source for intense, narrowband THz pulses at about 1.8 THz, the plasmon frequency was tuned via the grating-gate. The strongest pump-probe signals are observed at resonance, where a rather low pump fluence of about $200\,nJ/cm^2$ leads to a pump-induced change in transmission of more than 40% [1]. The signal decays within about 50 ps. The experimental results are complemented by a finite-difference time-domain electrodynamic simulation, allowing to identify the main driving mechanisms for the observed strong nonlinearity, e.g. near-field effects and hot charge carriers.

[1] P. Sai et al., Adv. Optical Mater. 2025, 13, 2500716; https://doi.org/10.1002/adom.202500716

HL 52.3 Fri 10:00 POT/0006

Plasmonic nonlinearity in AlGaN/GaN-based rectangular patches — •Nandita Bajpai[1], Pavlo Sai[2,4], Maksym Dub[2,4], Alexej Pashkin[3], Stephan Winnerl[3], Wojciech Knap[2,4], and Martin Mittendorff[1] — [1]Department of Physics, University of Duisbur-Essen,Duisburg,Germany — [2]Institute of HighPressure-Physics,Warsaw,Poland — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Center for Terahertz Sciences and Applications CENTERA -CEZAMAT Warsaw University of Technology, Warsaw, Poland

Recent observation of enhanced nonlinear THz absorption by resonant excitation of 2D plasmons in the AlGaN/GaN based plasmonic crystal has revealed a strong pump-induced transparency of probe upto 45%[1].Here, we investigate the nonlinear coupling between the perpendicular plasmonic modes in AlGaN/GaN-based rectangular patches. To this end, we performed a two colour pump probe experiment at the free-electron laser facility at the Helmholtz-Zentrum Dresden-Rossendorf. The spectrally narrow pump pulse was used to drive the plasmonic resonance at 1.95 THz whereas a broadband THz pulse from a synchronized table-top time domain spectroscopy setup was exploited to probe the plasmonic mode at 1.38 THz. We observed a relative pump - induced change in transmission of probe upto 12%, which is attributed to the excitation of hot carriers that decays within 25ps.

[1] P.Sai et al., Adv. Optical Matter.2025,13,2500716; https://doi.org/10.1002/adom.202500716

HL 52.4 Fri 10:15 POT/0006

Elucidating carrier dynamics in bismuth thin film with time-resolved terahertz spectroscopy — •Guriviredddy Yettapu, Fabian Thiemann, Michael Horn-von Hoegen, and Martin Mittendorff — University of Duisburg-Essen, Duisburg, Germany

Bismuth (Bi) is a Peierls distorted semimetal in its bulk state that transforms into a semiconductor for thicknesses below ~30 nm [1]. Time-resolved terahertz spectroscopy is an ideal tool to investigate the charge carrier dynamics by following the pump-induced change in electric field with pump-probe delay. Herein, we employed optical-pump terahertz-probe spectroscopy to elucidate the carrier dynamics in single crystalline Bi film with a thickness ~36 nm, including spectrally resolved measurements to determine the frequency dependent complex conductivity. At a pump fluence of 30 uJ/cm2, we observe a pump-induced change of the electric field of about 20 %, followed by an exponential decay with a relaxation time of ~7 ps. Our results reveal

that carrier relaxation times are hardly affected by the pump fluence, the complex conductivity can be well described by the Drude model. Our future studies include thickness- and temperature-dependent measurements to gain insights about the carrier-lattice interactions in the semiconductor and semimetal phase. [1] C. A. Hoffman et al., Phys. Rev. B. 48, 11431-11434 (1993).

HL 52.5 Fri 10:30 POT/0006

Identifying the semiconductor doping range addressable by terahertz time-domain spectroscopy — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Mirco Kutas[1,2], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department for Materials Characterization and Testing, Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Semiconductors are essential materials for the technological advancements of the 21st century. With the growing demand for semiconductor devices going along with this, the need for fast and non-destructive characterization techniques is growing quickly, too. Terahertz time-domain spectroscopy (THz-TDS) has proven to be capable of measuring the desired properties of various semiconductors over the last decades. Yet, it is still not widely established for this purpose. One reason is that for each combination of material, doping concentration and thickness the possibility to characterize the sample has to be evaluated individually. Therefore, we are developing a simulation-based tool that can help identify the accessible doping ranges. Based on simulations of the interaction between a terahertz pulse and an arbitrary layer stack of doped semiconductor materials, a well-founded estimate of the characterizability with reflection THz-TDS is retrieved. These simulations allow for a better understanding of the suitability of a THz-TDS characterization for specific semiconductor samples and hence to establish THz-TDS further in the semiconductor industry.

HL 53: Organic Semiconductors: Carrier Dynamics

Time: Friday 9:30–11:15 Location: POT/0051

Invited Talk HL 53.1 Fri 9:30 POT/0051

Organic semiconductors: Opening new perspectives in sustainable electronics — •Karl Leo — IAPP, TU Dresden

Organic semiconductors enable a variety of novel applications for flexible, lightweight, and environmentally friendly electronics. One unique advantage of these carbon-based materials is their compatibility with body tissue, thus opening perspetives for completely new medical applications on and even in the human body. Furthermore, the materials set available in this technology allows biodegradability and thus sustainable electronics without the serious environmental issue of conventional electronics. In the first part of my talk, I will show examples how organic electronic devices can be used in postsurgical monitoring, avoiding life-threatening complications. In the second part of the talk, I will address lignocellulose leaf skeleton structures (Leaftronics) as basis for a variety of novel applications, such as semitransparent electrodes.

HL 53.2 Fri 10:00 POT/0051

Unveiling the role of disorder on carrier concentration transients in electrochemical transistors — •Tobias Krebs and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Already the drain current transients in organic electrochemical transistors hint for not yet fully understood underlaying device physics, as they show a generally slower turn on compared to turn off, with the difference between these on- and off- switching times varying over orders of magnitude between materials and driving voltages. Tracking the charge carrier concentration during switching then completes this asymmetric picture: A sharp doping front entering the device during turn on, followed by gradual bulk de-doping during turn off. We measure these concentration transients optically, using the red-shifted absorption in the doped state of the redox active polymers we investigated. Comparison of this data with drift-diffusion simulations revealed a strong dependence of this asymmetry on the broadness of the density of states, which in our simulations both modulates the carrier density dependence of hole mobilities and influences the maximum charge carrier concentration for a set gate voltage. Our simulation framework also allowed us to study the surprisingly small effect of ionic mobilities in the semiconductor on switching times, above a device specific mobility threshold. The results can be used to guide the rational design of improved devices.

HL 53.3 Fri 10:15 POT/0051

Simulation of Coulomb Glass Behavior in Organic Semiconductor Devices at high carrier densities — •Magdalena Dörfler[1], Heinz Bässler[2], Anna Köhler[1,2], and Harald Oberhofer[3] — [1]Soft Matter Optoelectronics and Bayerisches Polymerinstitut (BPI), Experimental physics II, University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany — [3]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany

Recent advances in organic transistors (OFETs, EGOFETs, OECTs) enable device operation at high charge carrier densities where Coulomb interactions between carriers become significant.

Using Kinetic Monte Carlo simulations, we investigate carrier-carrier Coulomb interactions in OFET-like structures. Comparing simulations with and without these interactions reveals reduced carrier mobility and increased activation energy when interactions are included, with effects increasing for higher carrier densities.

Our results indicate a transition to correlated transport with a Coulomb gap in a dynamic density of states. The system exhibits Coulomb glass behavior, where the activation energy reflects structural reorganization of the carrier ensemble.

Notably, the Coulomb gap appears at ambient temperature and does not require variable-range hopping, unlike to the situation in electron liquids and inorganic semiconductors.

HL 53.4 Fri 10:30 POT/0051

Dual Ferroelectric and Semiconducting behaviour in supramolecular organics — •Tara Vollus[1], Sophia Klubertz[1], Shyamkumar Vadakket Haridas[2], Oleksandr Shysho[2], Max von Delius[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Germany — [2]Institute of Organic Chemistry, Ulm University, Germany

The combination of interacting conductive and ferroelectric properties, resulting in a multifunctional material, has the potential to simplify the structure of memory devices. It has been demonstrated that the organic ferroelectric material C6H6F5O-C3-amide (M3) exhibits both these properties, showing ferroelectricity and an unexpected DC conductivity.[1][2] It has been shown that the latter is related to the presence of interfacial dipoles that allow efficient charge injection from (oxidation and/or reduction by) metal contacts and is enhanced by a supramolecular arrangement formed at higher temperatures and under an applied electric field. Here, we demonstrate the effects of alignment and, especially, the presence of both n- and p-type doping-like processes, suggesting that M3 is a wide-bandgap organic semiconductor that reversibly can be reduced and oxidized. Kelvin probe force microscopy measurements revealed filament-like potential structures that may act as pathways for bipolar charge transport, and suggest the formation of dynamic pn-junctions.[3]

[1] Mager et al., arXiv:2507.11309 [cond-mat.mtrl-sci] [2] Mager et al., arXiv:2506.02673 [cond-mat.mtrl-sci] [3] Matyba et al., DOI:10.1038/nmat2478

HL 53.5 Fri 10:45 POT/0051

Backbone Alignment and Morphology Formation in PBTTT Thin Films: Insights from In-Situ GIWAXS — •Robin M. Teichgreber[1], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamics and Structure Formation - Herzig Group, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton

The performance of organic electronic devices strongly depends on the morphology of the organic semiconductor thin film [1]. Enhancing

the understanding on fundamental structure-function relationships is therefore crucial to improve the performance of such devices in the future. Highly aligned films can furthermore be used to study fundamental charge separation processes. Controlling the alignment of polymer backbones is a challenge in the first place, demanding further research on the processes of structure formation resulting in aligned films. Using PBTTT as a model system, the influence of different coating parameters on the kinetics of film formation during the deposition thin films via blade-coating is investigated by employing time-resolved in-situ GIWAXS measurements. Furthermore, the formation of high degrees of alignment during the post-deposition annealing process was studied with temperature-resolved GIWAXS. [1] Herrmann, N.J., von Coelln, N., Teichgreber, R.M., Höfener, S., Huck, C., Ghalami, F. et al. (2023) J. Mater. Chem. C, 11, 10185-10197.

HL 53.6 Fri 11:00 POT/0051

Multiscale Modelling of the Density of States in PEDOT:Tosylate Films — •Melissa Kim Meinel and Igor Zozoulenko — Laboratory of Organic Electronics, Linköping University, Norrköping, Sweden

A key descriptor of the electronic structure is the density of states (DOS), which directly affects properties such as charge mobility, intrinsic capacitance, and optical absorption. Structural disorder and the local electrostatic environment strongly influence the DOS but are rarely captured in full detail in computational studies that often rely on small model systems or simplified methods. We present a multiscale modelling approach for computing the DOS of realistic PEDOT:Tosylate films. Molecular dynamics simulations generate film structures that capture the complex packing and disorder of PEDOT chains and counterions. These configurations are analysed within a quantum mechanical/molecular mechanical (QM/MM) framework, where molecular mechanics accounts for large-scale heterogeneity while quantum calculations resolve local electronic states under explicit electrostatic embedding of the environment. Steric effects are treated at the MM level, while the QM region can be limited to a single chain. Accurate results require optimally tuned range-separated hybrid functionals, geometry optimisation of the QM chain, and iterative adaptation of charge distributions to capture realistic environmental effects. This framework enables quantitatively realistic, morphology-sensitive predictions of the electronic structure and has been applied to systems at different oxidation levels.

HL 54: 2D Materials IX – Photonic properties and devices

Time: Friday 9:30–12:45 Location: POT/0081

HL 54.1 Fri 9:30 POT/0081

Signature of interference between second and fourth order nonlinearities in atomically thin crystals — •Paul Herrmann[1], Jonas Margraf[1], Sebastian Klimmer[1], Sebastian Piehler[2], Maximilian Graml[2], Muhammad Sufyan Ramzan[3], Caterina Cocchi[3], Jan Wilhelm[2], and Giancarlo Soavi[1,4] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [3]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Jena, Germany — [4]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

Transition metal dichalcogenides (TMDs) are a well studied class of two-dimensional materials, whose opto-electronic properties are dominated by excitons and exhibit strong light-matter interaction. The relaxed phase matching in TMD monolayers facilitates the emission of many orders of nonlinearities with approximately equal efficiency. Thus, one can in principle observe interference effects between nonlinearities of different orders N (N=2,3,4,...). Here, we observe a previously unseen modulation of the generated second harmonic upon rotation of the input fundamental polarization. By combining wavelength and power dependent measurements with macroscopic, symmetry-based calculations and microscopic density functional theory simulations, we can assign this modulation to an interference between second and fourth order terms of the nonlinear polarization.

HL 54.2 Fri 9:45 POT/0081

Measurement of optically induced broken time-reversal symmetry in atomically thin crystals — •Florentine Friedrich[1], Paul Herrmann[1], Shridhar Shanbhag[2], Sebastian Klimmer[1], Jan Wilhelm[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany

Time-reversal symmetry (TRS) and space-inversion symmetry (SIS) are fundamental properties underlying phenomena like magnetism and non-trivial spin textures in crystals. Transition Metal Dichalcogenides (TMDs) offer a tunable platform to study the interplay of these symmetries, which can be engineered by tuning the number of layers and via all-optical bandgap modulation. We propose a powerful, all-optical approach using third harmonic (TH) Faraday rotation to probe broken TRS, regardless of the SIS [1]. By exciting mono- and bilayer TMDs with elliptically polarized light, we achieve spin-selective bandgap modulation, consequently breaking TRS. This symmetry reduction modifies the nonlinear susceptibility tensor, causing a measurable rotation of the emitted TH polarization. Our experimental results are supported by analytical theory for both mono- and bilayer TMDs and provide a unique tool to investigate spin, valley, and layer coupling in atomically thin semiconductors, thereby contributing to the understanding of the relation between crystal symmetries and the nonlinear optical response of a material.

[1] Friedrich et al., Nat. Photon., 10.1038/s41566-025-01801-2 (2025).

HL 54.3 Fri 10:00 POT/0081

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

Valleytronics explores the valley degree of freedom in materials like transition metal dichalcogenides (TMDs), using electrons in ±K valleys as binary states for information encoding. In valleytronics applications, efficient valley readout is crucial. We show that third harmonic generation (THG) provides an ultrafast solution to valley readout for both centrosymmetric and non-centrosymmetric materials [1].

We solved the semiconductor Bloch equations perturbatively to derive an analytical expression for the polarization state of the emitted third harmonic signal. Our analysis shows how material parameters influence the polarization and attributes polarization rotation to spin and valley dependent optical Stark and Bloch-Siegert shifts in TMDs. Our theoretical predictions closely align with experiments, providing the microscopic mechanism and thus helping advance valleytronic readout mechanisms.

[1] Friedrich, F., Herrmann, P., Shanbhag, S.S. et al. Nat. Photon. (2025). https://doi.org/10.1038/s41566-025-01801-2

HL 54.4 Fri 10:15 POT/0081

Nonlinear optical characterization of oxidized thin layered MoS2 — •Henry Hübschmann[1], Gerhard Berth[1], Klaus Jöns[1], Katharina Burgholzer[2], and Alberta Bonanni[2] — [1]Paderborn University, Paderborn, Germany — [2]Johannes Kepler University Linz, Linz, Austria

In the field of two-dimensional structures the class of transition metal dichalcogenides (TMDs) has sparked great interest in the last decades. Semiconductor materials like molybdenum disulfide (MoS2) have found many applications in photonic and optoelectronic devices [1,2]. An important characteristic is the tunability of the band structure and therefore consequently the possibility for modification of electronic and optical properties [3]. Within this work we conduct comprehensive second order nonlinear optical analysis on thermally oxidized mechanically exfoliated MoS2. In this context a layer number dependent investigation of the nonlinear response up to seven-layer configurations of AB-stacked 2H-MoS2 is performed. Here we found fingerprints of induced structural modifications identified which manifest themselves in

the strength of the nonlinear response and a resulting symmetry break of centrosymmetric media.

HL 54.5 Fri 10:30 POT/0081

quantum electrodynamics of excitons in bilayer graphene — •abraham nava mireles — the institut of photonic sciences, castelldefels, spain.

Cavity quantum electrodynamics has been a cornerstone in understanding light-matter interactions. In the so-called strong-coupling regime, these interactions cannot be described as a simple combination of their light and matter components. Instead, light and matter form new hybrid states. This project aims to push beyond into the ultrastrong coupling (USC) regime, where the interaction strength becomes comparable to the system's transition frequencies. In this regime, quantum vacuum fluctuations and elementary excitations become significant. This enables not only the control of quantum effects but also the modification of a material's ground state, even in the absence of external light. To that end, we explore the coupling between confined hyperbolic phonon polaritons (HPhPs) in hexagonal boron nitride (hBN) and excitons in bilayer graphene (BLG). The hyperbolic nature enables deep subwavelength confinement, enhancing the photonic density of states. In BLG, extended dipole transitions exhibit a nonlocal optical response, in which propagating HPhPs allow momentum-dependent transitions and access to a continuum of electronic final states. This leads to enhanced emission rates and to each exciton effectively coupling to multiple polaritonic modes, ultimately reaching a regime where the coupling strength compares to the transition frequency. This platform opens new possibilities for quantum technologies and non-perturbative light-matter engineering.

HL 54.6 Fri 10:45 POT/0081

All-TMDC nanobeam cavities with embedded $MoSe_2$ monolayers for enhanced light-matter interaction — •Aris Koulas-Simos[1], Pietro Metuh[2], Athanasios Paralikis[2], Kartik Gaur[1], Maximilian Klonz[1], Imad Limame[1], Chirag Palekar[1], Battulga Munkhbat[2], and Stephan Reitzenstein[1] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Berlin, Germany — [2]Department of Electrical and Photonics Engineering, Technical University of Denmark, Kongens Lyngby, Denmark

All-TMDC photonic structures enable enhanced light-matter interaction by combining high index contrast with atomically thin excitonic materials in a homogeneous platform [1]. Recent theoretical work [2] shows that all-TMDC nanostructures can support very large Purcell factors, highlighting their potential for nanoscale lasing. We realize WS_2 nanobeam cavities with a $MoSe_2$ monolayer embedded inside the dielectric cavity for improved field-exciton coupling compared to the conventional evanescent coupling schemes. Simulations predict a cavity mode at 766 nm with $Q \approx 4 \cdot 10^3$, a mode volume of approximately 2.6 $(\lambda/n)^3$, and a confinement factor $\Gamma \approx 0.8\%$. Cross-polarized reflectivity at room temperature reveals resonances between 725 and 760 nm with Q-factor values of 100-300, and low-temperature photoluminescence confirms coupling of the $MoSe_2$ monolayer to the cavity mode. These results establish a monolithic TMDC platform for future all-TMDC nanolasers and quantum emitters.

[1] B. Munkhbat et al., Laser Photon. Rev. 17, 2200057 (2023) [2] F. Binkowski, A. Koulas-Simos et al., arXiv:2508.05333 (2025), accepted

15 min. break or similar.

HL 54.7 Fri 11:15 POT/0081

Temperature-Dependent Moiré Polariton Formation in Bilayer MoSe2 Integrated in DBR based Microcavities — •Chirag Palekar[1], Aris Koulas-Simos[1], Imad Limame[1], Stephan Reitzenstein[1], and Bárbara Rosa[1,2] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]University of Campinas, R. Sérgio Buarque de Holanda, 777, 13085-636, Brazil

Twisted bilayer (tBL) MoSe2, which hosts moiré polaritons, when integrated into microcavities, provides a versatile platform for exploring light-matter interactions in moiré-engineered quantum materials. In the absence of the cavity, we observed the PL spectrum of the tBL exhibits multiple resonances corresponding to distinct moiré excitons. When embedded within a DBR cavity, such moiré excitons enter the strong coupling regime with the confined cavity photon mode, leading to the formation of moiré exciton-polaritons. Temperature-induced resonance tuning enables systematic control over the exciton-photon detuning, allowing modulation of the coupling strength. Remarkably, these moiré polaritons remain observable even at temperatures exceeding 150 K, underscoring the robustness of the hybridized light-matter states. Modeling the system using a coupled oscillator approach reveals a Rabi splitting as large as 11 meV. Our results demonstrate that temperature serves as an efficient external control parameter for engineering and tuning moiré exciton polaritons in twisted, atomically thin semiconductors, opening pathways toward reconfigurable polaritonic devices based on van der Waals heterostructures.

HL 54.8 Fri 11:30 POT/0081

Cavity polaritons in a hybrid van-der-Waals superconductor-semiconductor structure — •Seyma Esra Atalay, Hangyong Shan, Martin Esmann, and Christian Schneider — Carl von Ossietzky Universität Oldenburg, Germany

Monolayers of transition metal dichalcogenides (TMDs) offer new possibilities to study superconductivity. In this project, we investigate hybrid heterostructures of $NbSe_2/MoSe_2$ van der Waals layers, in the framework of cavity experiments. $NbSe_2$ and $MoSe_2$ are TMDs; superconductivity occurs in $NbSe_2$ [1], and the monolayer $MoSe_2$ is a direct band gap semiconductor that hosts excitons with high oscillator strength. By embedding the $NbSe_2/MoSe_2$ heterostructure in an open cavity [2], we achieve strong coupling between the $MoSe_2$ excitons and the cavity photons, forming exciton-polaritons, as evidenced by the pronounced Rabi gap seen in subsequent longitudinal and transversal cavity modes in where we tuned the open cavity length. This implementation of a hybrid superconductor-semiconductor monolayer polariton cavity forms the foundation of experiments to gain insight into how exciton-polariton coupling can influence the superconductive phase of $NbSe_2$ and allow us to further investigate optically tunable superconducting hybrid systems.

References [1]Xi, X., Wang, Z., Zhao, W. et al. Ising pairing in superconducting $NbSe_2$ atomic layers. Nature Phys 12, 139-143 (2016)., Journal 100, 101101 (2009) [2]J.C., Drawer et al., Nano Letters 2023 23 (18), 8683-8689

HL 54.9 Fri 11:45 POT/0081

Room temperature hybrid exciton-polaritons in a Perovskite-TMD heterostructrue — •Marti Struve[1], Hamid Pashaei Adl[1], Oliwia Janikwska[2], Sven Stephan[3], Jamie Fitzgerald[4], Paulina Plochocka[2,5], Christian Schneider[1], and Martin Esmann[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Wrocław University of Science and Technology, Wrocław, Poland — [3]University of Applied Sciences Emden, Emden, Germany — [4]Philipps-University Marburg, Marburg, Germany — [5]Laboratoire National des Champs Magnetiques Intenses, Toulouse, France

Chemically synthesized quasi-2D halide perovskites (HaP) exhibit strong excitonic resonances with large oscillator strength, high binding energy and tunable emission, making them an interesting platform for polariton physics at room temperature. Transition metal dichalcogenide (TMD), while showing lower oscillator strength, offer access to K-valley selective rules, opening the access to polarized excitonic states. In this work, we demonstrate the formation of hybrid exciton-polaritons in a quasi-2D HaP-TMD heterostructure embedded in a planar open cavity at room temperature. Using the tunability of our open cavity we first confirm strong coupling of our materials separately. When combined the system exhibits three polaritonic branches, showing a hybridization of the polariton modes that is reproduced using a three-oscillator Hamiltonian, revealing a state where both excitonic fractions become comparable. Our results lay the foundation to imprint the accessibility of the K-valley selection rules to HaP-polaritons devices leading to additional degrees of freedom.

HL 54.10 Fri 12:00 POT/0081

Tunable Room-Temperature Polaritons Achieving the Very Strong Coupling Regime in Quasi-2D Layered Perovskites — •Hamid Pashaei Adl[1], C. Bennenhei[1], M. Struve[1], P. Peksa[2], M. Dyksik[2], M. Baranowski[2], K. W. Song[3], M. Gittinger[1], C. Lienau[1], J. K. König[4], J. M. Fitzgerald[4], N. P. Jasti[5], F. Eilenberger[6], P. Plochocka[2], E. Malic[4], O. Kyriienko[7], M. Esmann[1], and C. Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany. — [2]Wroclaw University of Science and Technology, Wroclaw, Poland. — [3]Xiamen University Malaysia, Sepang, Malaysia. — [4]Philipps-Universität, Marburg, Germany. — [5]JNCASR, Bangalore, India. — [6]Max Planck School of Photonics, Jena, Germany. — [7]University of Sheffield, UK.

Layered halide perovskites are organic and inorganic 2D or quasi-2D

layers, which self-assemble in solution realizations of quantum well stacks with giant exciton oscillator strengths, tunable emission spectra and very large exciton binding energies. In this contribution, we discuss widely tunable room-temperature cavity exciton polaritons at the cross-over from the strong coupling to the very strong coupling regime, in mechanically exfoliated quasi-2D Ruddlesden-Popper iodide perovskite integrated into an open microcavity. We gradually increased the cavity length and observed a pronounced anti-crossing behavior associated with successive longitudinal cavity modes. The Rabi splitting exhibited a systematic reduction with increasing cavity length; however, the scaling behavior deviated from the conventional square root dependence typically observed in the strong coupling regime.

HL 54.11 Fri 12:15 POT/0081

Optical Gain in Lasers Based on Two-Dimensional TMD Semiconductors — Tommy Schulz[1], •Daniel Erben[1], Alexander Steinhoff[2], Weng Chow[3], and Frank Jahnke[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Institute for Physics, Faculty V, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany — [3]Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

We present a direct comparison of the optical gain in InGaAs quantum wells (QWs) and transition-metal dichalcogenide (TMD) monolayers on SiO_2 and encapsulated in hBN. A central objective of this work is to theoretically quantify the gain and to identify its microscopic origin. As a result, we find a substantially larger magnitude of the gain in TMDs - especially in WS_2 - and comparable transparency carrier densities in both systems. The enhanced interband Coulomb interaction in TMDs provides this superior gain performance, although the valley-rich conduction band makes sustaining population inversion more challenging than in InGaAs/GaAs QWs. Encapsulating WS_2 in hBN - a common approach to improve optical quality - proves advantageous, as it reduces carrier drain into side valleys, which lowers the transparency carrier density compared with WS_2/SiO_2. Lastly, we investigate the Henry factor (α), which governs key laser properties such as linewidth behaviour. InGaAs QWs exhibit large α values near transparency, hBN-encapsulated WS_2 shows weakly negative values - an indication towards more favourable lasing performance.

HL 54.12 Fri 12:30 POT/0081

Room-temperature polariton condensate in a quasi-2D hybrid perovskite — M. Struve[1], C. Bennenhei[1], H. Pashaei Adl[1], K.W. Song[2], H. Shan[1], N. Matukhno[1], J.-C. Drawer[1], S. Stephan[1], F. Eilenberger[3], N.P. Jasti[4], D. Cahen[4], O. Kyriienko[5], C. Schneider[1], and •M. Esmann[1] — [1]Carl von Ossietzky Universität Oldenburg — [2]Xiamen University, Sepang, Malaysia — [3]Frauenhofer IOF, Jena — [4]Weizmann Institute of Science, Rehovot, Israel — [5]University of Sheffield, UK

Quasi-2D halide perovskites are chemically synthesized quantum well stacks with large exciton oscillator strength and binding energy. Although promising for polaritonics, bosonic condensation and polariton lasing have so far remained elusive in quasi-2D perovskites at ambient conditions. Here, we demonstrate room-temperature cavity exciton-polariton condensation in mechanically exfoliated crystals of $(BA)_2(MA)_2Pb_3I_{10}$ in an in-situ tunable optical microcavity [1]. We observe a polariton condensation threshold of 0.41 μJcm^{-2} per pulse and detect a strong non-linear response. Interferometric measurements confirm the spontaneous emergence of spatial coherence across the polariton condensate. Our results lay the foundation for a new class of room-temperature polariton lasers based on quasi-2D halide perovskites with great potential for hetero-integration with other vander-Waals materials, photonic crystals and waveguides.

[1] M. Struve et al. arXiv:2408.13677 (Nat. Comms. accepted 2025)

HL 55: Quantum Dots and Wires: (Single) Photonics

Time: Friday 9:30–12:30 Location: POT/0251

HL 55.1 Fri 9:30 POT/0251

Fabrication of a III/V SiO2/SiN hybrid cavity incorporating a single Stark tunable (In,Ga)As quantum dot for high rate single photon generation — •Imad Limame, Kartik Gaur, Sarthak Tripathi, Setthanat Wijitpatima, Aris Koulas-Simos, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Institute for Physics and astronomy, Technical University of Berlin, Berlin, Germany

The advancement of quantum photonic technologies, particularly secure communication based on semiconductor quantum dots (QDs), relies on the on-demand generation of high-quality quantum light. Emission of single photons with high brightness, purity, and indistinguishability is essential for scalable quantum networks. However, the photon emission rate of QDs is fundamentally limited by their nanosecond-scale radiative lifetime. To overcome this, QDs are integrated into photonic nanostructures that enhance light-matter interaction via the Purcell effect, accelerating emission dynamics. Yet, such approaches often require complex bonding and alignment, hindering scalability.

We demonstrate a scalable hybrid cavity platform integrating a Stark-tunable QD within a p-i-n diode into a resonator composed of an epitaxially grown III-V bottom mirror and a PECVD-deposited dielectric top DBR. Deterministic QD positioning using marker-based EBL ensures precise spatial and spectral alignment, improving photon extraction and reducing the radiative lifetime. This approach enables scalable, high-brightness, coherent quantum light sources, providing a solid foundation for next-generation integrated quantum photonics.

HL 55.2 Fri 9:45 POT/0251

Deterministic single-photon source with on-chip GHz acoustic clock — •Alexander Kuznetsov[1], Meysam Saeedi[1], Zixuan Wang[2], Kevin Silverman[2], and Klaus Biermann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]National Institute of Standards and Technology, Boulder, Colorado 80305, USA

Solid state single-photon sources are a key component in quantum communication. Their efficiency depends strongly on the single-photon (SP) emission rates. Typically, the latter can be enhanced via Purcell effect by embedding quantum dots (QDs) in optical microcavities (MC), which requires the energy matching between MC optical mode and QD energies. Here, we demonstrate triggering of QD SP emission using dynamic Purcell effect induced by acoustic strain at a frequency of several GHz. To this end, InAs QDs are integrated in a hybrid photon-phonon AlGaAs microcavity, where the density of optical states is tailored by the lateral confinement of photons in umsized traps defined lithographical patterning of the microcavity spacer. We demonstrate modulation of QD energy up to 14 GHz using quasi-monochromatic strain of a piezoelectrically excited bulk acoustic wave. The modulation periodically shifts the QD transition in resonance with a spectrally narrow confined optical mode, leading to an enhancement of emission, i.e., the dynamic Purcell effect. In combination with high-Q MCs this approach is promising for SP rates above 10 GHz under continuous wave optical excitation. [arXiv:2510.22826]

HL 55.3 Fri 10:00 POT/0251

Beyond-Dipole Radiative Lifetimes of Excitons and Biexcitons in GaAs/AlGaAs Quantum Dots — •Petr Klenovský — Masaryk University, Brno, Czech Republic — Czech Metrology Institute, Brno, Czech Republic

Semiconductor quantum dots are promising sources of on-demand single and entangled photons, but a quantitative microscopic description of their radiative lifetimes remains challenging. We theoretically investigate Coulomb-correlated multi-particle states (X^0, $X^{\pm}$, XX) in weakly confining GaAs/AlGaAs quantum dots using an 8-band $\mathbf{k}\cdot\mathbf{p}$ model combined with continuum elasticity and configuration interaction (CI). Polarization-resolved oscillator strengths and radiative rates are computed both in the dipole approximation and in a quasi-electrostatic beyond-dipole formulation based on a Poisson reformulation of the dyadic Green tensor. For the dots studied, the beyond-dipole treatment yields exciton and biexciton lifetimes in quantitative agreement with experiment. We further analyze electric-field tuning of the multi-particle spectrum and the resulting indistinguishability, characterized by $P = \tau^X/(\tau^X + \tau^{XX})$, and discuss the sensitivity to CI-basis size and to electron-electron and hole-hole exchange.

HL 55.4 Fri 10:15 POT/0251

High-quality single photons from cavity-enhanced biexciton-to-exciton transition — •Nils Heinisch[1], Francesco Salusti[1], Timon L. Baltisberger[2], Mark R. Hogg[2], Malwina A. Marczak[2], Rüdiger Schott[3], Sascha R. Valentin[3], Andreas D. Wieck[3], Arne Ludwig[3], Klaus D. Jöns[1], Richard J. Warburton[2], and Stefan Schumacher[1] — [1]Department of Physics, CeOPP, and PhoQS, Paderborn University, Germany — [2]Department of Physics, University of Basel, Switzerland — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Generating high-quality photons using the biexciton-exciton cascade benefits from the separability of the photons from the two-photon excitation laser pulse. However, the intrinsic lifetime ratio between biexciton (XX) and exciton (X) states leads to a fundamental limit for the achievable indistinguishability of the single photons [1]. Therefore, the XX must decay much faster than the X. We achieve this with an optical resonator that resonantly enhances the XX-X transition. By optimizing the cavity parameters and avoiding phonon-mediated cavity feeding, we show that high-quality cavity photons originating from XX can be generated. Furthermore, we show that spectral filtering restores single-photon quality in regimes of XX binding energies, where X emission into the cavity is not initially excluded. Our theoretical investigations are joined by key results from the experimental demonstration, which make this approach a major advance in the realization of practical quantum light sources. [1] E. Schöll et al., PRL 125, 233605 (2020). D. Bauch et al., Adv. Quantum Technol. 7, 2300142 (2024).

HL 55.5 Fri 10:30 POT/0251

Photon-mediated electron capture into a single quantum emitter — •Daniel Oppers[1], Hendrik Mannel[1], Luca Henrichs[1], Fabio Rimek[1], Arne Ludwig[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

Single-photon emitters are one of the key components of quantum information technology. Especially single self-assembled quantum dots in a p-i-n diode structure for charge control are still a promising candidate. We use an InAs/GaAs quantum dot in a bias regime, where the dot is uncharged and drive the exciton transition optically resonant with a cw diode laser. A second off-resonant cw laser with a lower energy than any optical transition is used to induce an internal photoeffect [1], exiting electrons from the electron reservoir in the diode, that are captured into the quantum dot. Consequently, we observe a quenching of the exciton transition, which can no longer be driven resonantly. This electron capture by photo-excitation of electrons from the reservoir (see also [2]) is measured here in real-time, observing every quantum jump from an uncharged to a charged quantum dot in a random telegraph signal. Evaluating the telegraph signal using waiting time distributions we observe a linear increase in the electron capture rate scaling up with increasing excitation power of the off-resonant laser. Our findings reveal that photo-induced quenching is a possible source of exciton dephasing. [1] P. Lochner et. al., Phys. Rev. B **103**, 075426 (2021) [2] A. Kurzmann Appl. Phys. Lett. **108**, 263108 (2016)

HL 55.6 Fri 10:45 POT/0251

Influence of the internal photoelectric effect on the indistinguishability of single quantum dot photons — •Luca Henrichs[1], Fabio Rimek[1], Hendrik Mannel[1], Daniel Oppers[1], Arne Ludwig[2], Martin Geller[1], and Axel Lorke[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A single self-assembled quantum dot (QD) is one of the promising candidates as a bright (high photon rate) and stable (Fourier-limited) linewidth single photon source [1]. For applications in photonic devices or in quantum communication networks the dephasing process is an important property, where besides spin- and charge noise, the Auger-Meitner [2] and the photoeffect [3] could play an important role.

Here, we investigate the impact of the internal photoelectric effect on the indistinguishability of single QD photons. We used pulsed Hong-Ou-Mandel measurements at different excitation intensities of the exciton transition to determine the photon indistinguishability in various driving regimes, ranging from coherent scattering (the Heitler regime) to the incoherent regime above the saturation intensity. Above saturation, we observe the influence of the photoeffect, which reduces the indistinguishability. Our findings represent an important step toward understanding the decoherence of single photons in this important quantum system.

[1] N. Tomm et al., Nat. N. **16**, 399*403 (2021). [2] H. Mannel et al., AIP, **15**, 134 (2023). [3] P. Lochner et al, PR, **7**, 103, (2021).

15 min. break

HL 55.7 Fri 11:15 POT/0251

An ultra-compact deterministic source of maximally entangled photon pairs — Moritz Langer[1], Pavel Ruchka[2], Ahmad Rahimi[1], Sara Jakovljevic[2], Yared G. Zena[1], Sai Abhishikth Dhurjati[1], Alexey Danilov[1], Mandira Pal[1], Riccardo Bassoli[3], Frank H. P. Fitzek[3], Oliver G. Schmidt[4], Harald Giessen[2], and •Caspar Hopfmann[1,2] — [1]Institute for Emerging Electronic Technologies, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [3]Deutsche Telekom Chair of Communication Networks, Technische Universität Dresden, Dresden, Germany — [4]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

We demonstrate an ultra-compact source of on-demand, maximally entangled photon pairs using single GaAs quantum dots in monolithic microlenses, efficiently fiber-coupled in a cryogenic environment. A 3D-printed micro-objective facilitates near-diffraction-limited performance at 3.8 K. The system achieves high single-photon emission rates (392(20) kHz) and purities (0.992(5)) via two-photon resonant excitation. Leveraging the exciton-biexciton cascade, it produces near-maximally entangled photon pairs (peak entanglement negativities of 2n=0.96(2)). This quantum light source combines state-of-the-art performance and stability with a dramatically reduced footprint, well-suited for seamless industrial integration.

HL 55.8 Fri 11:30 POT/0251

Spectral shadows of a single GaAs quantum dot — •Jens Hübner[1], Kai Hühn[1], Lena Klar[1], Fei Ding[1], Arne Ludwig[2], Andreas D. Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Semiconductor quantum dots are today's leading candidates for generating single and entangled photons. However, even the most advanced devices face performance limitations due to charge state fluctuations within the quantum dot and its surrounding environment. We have carried out detailed time-resolved resonance fluorescence measurements on an individual charge-tunable GaAs quantum dot, providing new insight into the spectral signatures generated by the complex landscape of unintentional impurities. For the neutral exciton and the negatively charged trion transitions, we uncover multiple Stark-shifted resonances, linked to rare spectral jumps smaller than the homogeneous linewidth. In other experiments, these jumps are typically obscured by measurement noise. In contrast, the positively charged and doubly negatively charged trions exhibit distinctly different behaviors. We quantify the underlying impurity charge dynamics over timescales ranging from sub-milliseconds to several seconds, and demonstrate that the hole population of the positively charged trion is limited in our state-of-the-art pin-structure by fast hole loss combined with slow hole recapture.
[Hühn et al., arXiv:507.20290 (2025)]

HL 55.9 Fri 11:45 POT/0251

Adhesive bonding of In(Ga)As - QD membrane on Silicon for evanescent light coupling — •J. Unfried[1], R. Vijayan[1], U. Pfister[1], D. Wendland[2], S. Oberle[1], M. Weiss[1], M. Jetter[1], S. Portalupi[1], and P. Michler[1] — [1]IHFG, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]AG Pernice, Universität Münster, Heisenbergstraße 11, 48149 Münster, Germany

Hybrid integration of III-V materials with silicon photonics involves combining efficient III-V light emitters with low-loss, CMOS-compatible Si platforms. This allows high-performance PICs to be realised. Adhesive bonding is a scalable and flexible method for achieving this integration. It provides and enables lithography-defined alignment. However, this approach also presents significant challenges. Efficient coupling between the III-V active membrane and Si waveguides (WG) requires an extremely thin, optically transparent bonding layer to enable strong evanescent coupling. Such thin layers restrict the thermal budget available for post-bonding processes, and may result

in delamination during subsequent fabrication steps. Reliable integration therefore necessitates an optimised bonding process and carefully controlled fabrication conditions. This work focuses on integrating an InGaAs membrane with C-band InAs QDs onto a Si photonic platform using an optimised adhesive bonding scheme. A simulation-guided design approach is employed to identify suitable waveguide and taper geometries, and a reproducible bonding process is used to fabricate uniform, thin bonding layers and tapered InGaAs waveguides that efficiently couple QD emission into Si waveguides.

HL 55.10 Fri 12:00 POT/0251

Revisiting Quantum Well Thickness Fluctuation Quantum Dots as a Source of Single Photons — •Tom Fandrich[1], Frederik Benthin[1], Yiteng Zhang[1], Benjamin Bohn[1], Maximilian Heller[1], Johan Hilbig[1], Tom Rakow[1], Arijit Chakraborty[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover

Semiconductor-based quantum dots (QDs) are promising candidates for quantum network applications due to their ability to generate single, entangled, and indistinguishable photons on demand. Modern epitaxial III-V quantum emitters based on local droplet etching with nanohole infilling or Stranski-Krastanov growth exhibit excellent properties from the near-infrared to the telecom bands. An alternative from the early days of QD research involved QDs formed by thickness fluctuations in quantum well (QW) heterostructures. These QW thickness fluctuation (QWTF) QDs can naturally display strong light-matter interaction due to giant oscillator strengths, yet have not been the focus of recent research as quantum emitters for single-photon applications. In this work, we investigate the optical properties of naturally formed QWTF QDs in GaAs QWs emitting near 780 nm. Our results demonstrate that their distinctive properties justify revisiting QWTF QDs with today's standard for single-photon sources competiting against state-of-the-art epitaxial approaches.

HL 55.11 Fri 12:15 POT/0251

Single-Photon Emission with High Spectral Purity from Site-Controlled InGaN Quantum Dots — •Nima Hajizadeh[1,2], Nils Bernhardt[2], Richard Zimmermann[2], Felix Nippert[2], Luca Sung-Min Choi[2], Benjamin Damilano[3], Jean-michel Chauveau[4], and Markus Wagner[1,2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V. — [2]Technische Universität Berlin, Institute of Solid State Physics — [3]Université Côte d'Azur, CNRS, CRHEA — [4]Université Paris Saclay, Université Versailles Saint Quentin, CNRS, GEMaC

The development of high-quality Single-Photon Emitters (SPEs) based on Indium Gallium Nitride (InGaN) Quantum Dots (QDs) is essential for advancing quantum technologies. We present a comprehensive investigation of SPEs based on novel top-down fabricated, site- and size-controlled InGaN QDs. In this work, the optical and quantum optical properties of these isolated QDs are comprehensively investigated using high-resolution, time-correlated micro-photoluminescence (μ-PL) spectroscopy, including temperature-, power- and polarization-dependent measurements, as well as hyperspectral PL mapping of their excitonic emission. The purity of the single-photon emission is evaluated by measuring the second-order intensity autocorrelation function $g^{(2)}(\tau)$ in a Hanbury-Brown and Twiss (HBT) setup. We show that the emitter exhibits an exceptionally sharp emission bandwidth below 0.02 nm and pronounced antibunching with $g^{(2)}(0) < 0.36$. These results confirm the potential of our site-controlled growth methodology to deliver high-purity SPEs with narrow spectral lines.

HL 56: Quantum Emitters in 3D Semiconductors

Time: Friday 11:15–12:30 Location: POT/0006

HL 56.1 Fri 11:15 POT/0006

Electrically driven single-photon sources for scalable quantum photonics operating at the telecommunication wavelengths — •Alessandro Puddu[1,2], Junchun Yang[2], Shengqiang Zhou[1], Artur Erbe[1,2], Ahmad Echresh[1], Kambiz Jamshidi[2], and Yonder Berencén[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01069, Germany

Silicon-based quantum technologies provide a scalable platform for photonics due to their CMOS compatibility and ease of integration. Single-photon sources operating at telecom wavelengths are key components for low-loss quantum communication networks and the emerging quantum internet. Integrating these emitters with reconfigurable photonic elements such as multiplexers, modulators, filters, etc. and on-chip single-photon detectors is essential for realizing scalable quantum hardware. Optical excitation methods, however, rely on complex and alignment-sensitive laser systems, limiting their integration potential. Electrically driven color centers offer a compact and fully integrable alternative. This paper is focused on achieving electrically driven single-photon emission from individual color centers embedded in a silicon PIN diode. Emission in the telecom O- and L-bands is particularly advantageous, as it aligns with low-loss and low-dispersion regions in standard optical fibers. To improve emission efficiency and on-demand single photon generation, a single-color center will be coupled to a CMOS-compatible optical cavity, enabling Purcell-enhanced emission and efficient integration into silicon photonic circuits.

HL 56.2 Fri 11:30 POT/0006

Liquid Metal Alloy Ion Sources for Quantum Emitters — •Nico Klingner[1], Lukas Prager[1], Gregor Hlawacek[1], Stefan Findeisen[1], Wolfgang Pilz[2], and Paul Mazarov[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany

Liquid metal alloy ion sources (LMAIS) have evolved into powerful emitters for generating focused ion beams (FIBs) of a wide range of elemental species. In recent years, they have become a key enabling tools for quantum technologies, supporting applications such as deterministic single-ion implantation, the controlled creation of defect centers acting as single-photon sources, or for local isotopic purification of silicon for quantum-grade materials.

In this contribution, we present an overview of the LMAIS fabrication process, inluding eutectic alloy phase diagrams in selecting suitable compositions, the microfabrication and sharpening of emitter needles, and the challenges of alloy wetting and reservoir filling. As the alloy chemistry and emitter surface are highly susceptible to contamination, all steps are recently carried out under ultra-high-vacuum conditions to prevent oxidation and ensure reproducible operating characteristics.

Finaly we will show a summary and an outlook on single photon emitter production that benefit from the unique versatility of LMAIS-based ion beams.

HL 56.3 Fri 11:45 POT/0006

Defect-based quantum emitters in aluminum nitride — •Annkathrin Köhler, Jan Böhmer, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Aluminum nitride (AlN) has recently gained attention as a promising platform for integrated quantum photonic applications, where single-photon emitters (SPEs) play a key role in quantum communication and on-chip information processing. Its wide bandgap, CMOS compatibility, and established role in optoelectronic technologies make AlN an attractive host for stable, room-temperature SPEs. However, the microscopic origin and controllability of its defect-based emission remain insufficiently understood, challenging the implementation in scalable quantum photonic devices. Here, we investigated the defect-related luminescence in commercially available PVD-grown AlN thin films using micro-photoluminescence spectroscopy and second-order correlation measurements. By characterizing both intrinsic defects and extrinsic impurities introduced through controlled ion irradiation, we aim to identify routes toward reproducible and deterministic creation of optically active defect centers. Ion irradiation provides a tunable method for introducing specific defect types and spatially localized emitters, potentially enabling on-demand SPE fabrication. This study supports

the development of AlN as a viable wide-bandgap host for quantum light sources and outlines directions for integrating AlN-based SPEs into future photonic architectures.

HL 56.4 Fri 12:00 POT/0006

Atomic force lithography positioned circular Bragg cavities for high performance quantum dot based quantum light sources. — •Abhishikth Dhurjati[1], Moritz Langer[1], Yared Zena[1], Ahmad Rahimi[1], Liesa Raith[1], Martin Bauer[1], Riccardo Bassoli[2], Frank Fitzek[3], and Caspar Hopfmann[2] — [1]Institute for Emerging Electronic Technologies, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Quantum Communication Networks research group, Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany — [3]Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany

Semiconductor quantum dots (QDs) are excellent quantum emitters, but their random spatial distribution hinders deterministic cavity integration. We present a room-temperature atomic force microscopy (AFM) assisted nano-oxidation technique enabling deterministic QD positioning with a radial displacement of 51(28) nm. Free-standing circular Bragg gratings fabricated around positioned GaAs QDs exhibit a 245-fold photoluminescence enhancement and fine-structure splitting comparable to bulk QDs. Polarization-resolved measurements and simulations show robust cavity-coupled emission for in-plane displacements up to 50 nm and devices with Stokes imbalance below 5 percent, confirming precise alignment and a scalable route toward high-performance quantum light sources.

HL 56.5 Fri 12:15 POT/0006

Bright quantum dot light sources using monolithic microlenses on gold back-reflectors — •Moritz Langer[1,2,3], Sai A Dhurjati[1], Yared Zena[1], Ahmad Rahimi[1], Mandira Pal[1], Liesa Raith[1], Sandra Nestler[1], Riccardo Bassoli[2,3], Frank H P Fitzek[3], Oliver G Schmidt[4], and Caspar Hopfmann[1,2,3] — [1]Institute for Emerging Electronic Technologies - IFW Dresden, Dresden, Germany — [2]Quantum Communication Networks Research Group, Dresden University of Technology, Germany — [3]Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany — [4]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Germany

We present a scalable approach for fabricating bright GaAs quantum-dot photon sources by integrating QDs into broadband monolithic AlGaAs microlens arrays on gold-coated GaAs substrates. Thermally reflowed photoresist templates are transferred into AlGaAs thin films using an optimized 3D reactive-ion etching process, enabling large-area arrays with highly uniform lens geometries. Photoluminescence statistics reveal brightness enhancements of up to *200, occurring in roughly 1 out of 200 lenses, in good agreement with our developed fabrication-yield model. Finite-difference time-domain simulations predict extraction efficiencies of up to 62% for free-space collection and 37% for fiber-coupling. These results highlight the strong potential of this platform for compact, scalable entangled-photon sources in future quantum networks.

HL 57: Nitrides IV – Optical properties

Time: Friday 11:30–12:45 Location: POT/0051

HL 57.1 Fri 11:30 POT/0051

Optical Properties of Sn-doped n-type GaN — •Hannah Bendin[1], Elias Kluth[1], Kazuki Ohnishi[2], Kansuke Hamasaki[2], Shugo Nitta[2], Naoki Fujimoto[2], Hirotaka Watanabe[2], Yoshio Honda[2], Hiroshi Amano[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Otto-von-Guericke-Universität Magdeburg, Germany — [2]Nagoya University, Japan

GaN is at the heart of many contemporary electronic and optoelectronic applications. To increase the efficiency of high-power devices, the preparation of degenerately doped n-type GaN of high quality is required. Generally, Si and Ge are introduced as dopants, each giving rise to their own challenges. For example, high Si-doping is counteracted by carrier compensation and an increase in tensile stress. Recently, Sn has also gained interest as a dopant in GaN. Initial theoretical and experimental studies show promising results, introducing Sn as a candidate for strain control in n-type GaN via co-doping with Si or Ge, as the radius mismatch between Ga and Sn causes compressive strain, unlike Si or Ge. Here, we investigate Sn-doped samples with different carrier concentrations grown by halide vapor phase epitaxy by employing a variety of optical techniques. To determine the influence of the carrier concentration in GaN:Sn on the optical properties, we apply spectroscopic ellipsometry, Raman spectroscopy, and photoluminescence. Two sets of samples have been investigated: (I) GaN:Sn on a GaN/sapphire template and (II) GaN:Sn on a freestanding GaN substrate.

HL 57.2 Fri 11:45 POT/0051

Optical properties of ScAlN: investigation by spectroscopic ellipsometry — •Christina Harms[1], Jona Grümbel[1], Duc V. Dinh[2], Zhuohui Chen[3], Oliver Brandt[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität, Institut für Physik, Magdeburg, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Huawei Technologies Canada Co., Ltd., Kanata, Canada

$Sc_xAl_{1-x}N$ alloys are of increasing interest due to their unique ferroelectric and optoelectronic properties. In this work, we investigate the dielectric function of this material using spectroscopic ellipsometry. A series of $Sc_xAl_{1-x}N$ samples with $0 \leq x \leq 0.35$, grown on AlN/Si by plasma-assisted molecular beam epitaxy, were measured in the infrared (IR) and ultraviolet (UV) spectral range. In the IR range, the E_1(TO) phonon mode is characterized in terms of its resonance frequency ω and broadening γ, which are analyzed as a function of Sc content. Additionally, the dielectric limit ε_∞ is derived. With increasing Sc content, ω decreases, while both γ and ε_∞ increase. In the UV range, we determine the optical bandgap E_g as well as the corresponding ε_∞ and describe the observed trends across the composition range. Here, E_g decreases systematically with increasing Sc content and ε_∞ increases accordingly. The results are compared with recent results from literature, showing consistent trends in the optical properties throughout the investigated composition range.

HL 57.3 Fri 12:00 POT/0051

Near-lattice-matched AlScN/GaN heterostructures studied by spectroscopic ellipsometry and photoluminescence — •Alwin Wüthrich[1], Rajendra Kumar[2], Oana Malis[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department of Physics and Astronomy, Purdue University, USA

Understanding the fundamental properties of the novel ferroelectric material AlScN, such as ferroelectricity, tunable lattice constants, a wide and tunable band gap, and high piezoelectric coefficients, is crucial for its correct implementation in modern applications. Examples include processing units based on non-volatile memory and the design of infrared devices that utilize transitions between strongly confined electronic states, i.e., intersubband transitions. Here, near-lattice-matched AlScN layers (with 4–25% Sc) were grown by molecular beam epitaxy (MBE) on MBE-grown GaN layers. The samples were investigated by spectroscopic ellipsometry from the near-infrared to the far-ultraviolet range, probing infrared-active phonons and interband transitions. Additionally, the samples were studied by temperature-dependent photoluminescence, revealing luminescence from a two-dimensional electron gas.

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Near-Infrared Photocurrent Spectroscopy of InN Two-Terminal Devices — •Alexandra V. Nemmaier[1,2], Maximilian A. Gruber[1,2], Abhilash Ulhe[1,2], Gregor Koblmüller[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Exzellenzcluster e-conversion, Munich, Germany

The semiconductor InN, with its narrow bandgap, high electron mobility, and specific carrier cooling mechanisms, is a promising platform

for optoelectronics and hot carrier solar cells. We investigate epitaxial InN layers grown on GaN by near-infrared photocurrent spectroscopy. We measure the spatially resolved photocurrent to characterize the photoresponse in gated two-terminal devices. This approach offers a new perspective on hot carrier generation, charge carrier transport, and relaxation mechanisms close to the bandgap of the material.

HL 57.5 Fri 12:30 POT/0051

Structural and vibrational properties of strain-free $Al_{1-x}Sc_xN$ nanowires — Adriano Notarangelo[1], Ileana Florea[2], Philippe Vennéguès[2], Aidan Campbell[1], Hans Tornatzky[1], Jonas Lähnemann[1], Thomas Auzelle[1], Lutz Geelhaar[1], Oliver Brandt[1], and •Philipp John[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V. 10117 Berlin, Germany — [2]Université Côte d'Azur, CRHEA, CNRS, 06905 Sophia-Antipolis Cedex, France

The incorporation of Sc into the wurtzite crystal lattice of AlN enhances its piezoelectricity and induces ferroelectricity, making $Al_{1-x}Sc_xN$ an attractive material for novel types of group-III nitride based devices. Yet, the lattice distortions giving rise to these functionalities are superimposed to distortions arising from residual strain introduced during the heteroepitaxy on lattice-mismatched substrates.

In this work, self-assembled wurtzite $Al_{1-x}Sc_xN$ nanowires are grown by molecular beam epitaxy, varying the Sc content x from 0 to 0.38. The nanowire geometry allows elastic relaxation to occur, resulting in strain-free, bulk-like $Al_{1-x}Sc_xN$. A non-linear evolution of lattice parameters and a continuous red-shift of the E_2^{high} and $A_1(TO)$ phonon modes as a function of Sc content are found, confirming its incorporation into the wurtzite lattice and revealing modifications of anion-cation bond strength and coordination environment.

Our results highlight the advantages of bulk-like $Al_{1-x}Sc_xN$ for probing its fundamental properties, laying the ground work for further device applications.