HL 36: Poster III

Topics:
- 2D semiconductors and van der Waals heterostructures
- Functional semiconductors for renewable energy solutions
- Nanomechanical systems for classical and quantum sensing
- Nitrides

Time: Wednesday 18:00–20:30 Location: Poster E

HL 36.1 Wed 18:00 Poster E

Entangled two-photon absorption in 2D semiconductors — •Till Weickhardt and Giancarlo Soavi — Institute of Solid State Physics, Jena, Germany

The excitonic states in TMDCs lead to resonant enhancement of SHG and two-photon absorption (TPA) with huge cross-sections and have been proposed as gates for valleytronics.[1] To generate detectable populations of excitons in two photon processes with classical light and not damaging the monolayer it is necessary to use a pulsed laser with a broad spectrum. This limits the energy resolution of any experiment. In this work, we propose a possible way to remedy this problem by using energy-time entangled photons from spontaneous parametric down conversion (SPDC). This way, the photons are temporally synchronized in pairs and sum up to a precise and narrow energy spectrum while the distribution of single-photon energies can be broad.[2] This leads to higher efficiencies for TPA combined with spectral resolution beyond the Fourier limit. Entangled two-photon absorption (ETPA) has been demonstrated in fluorophores but never in solid-state systems.[3] To achieve this, two experimental requirements must be met: (i) a tunable narrowband laser to precisely hit the excitonic resonances of the TMDC under investigation. (ii) a SPDC source with high photon-pair flux, leading to an average power of at least 100 nW. While these requirements have already been met in our labs, first measurements of ETPA in TMDCs are still pending at this stage.

References: [1]Herrmann et al., Small 19, 2301126(2023) [2]Dayan et al., PRL 94, 043602(2015) [3]Tabakaev et al., PRA 103, 033701(2021)

HL 36.2 Wed 18:00 Poster E

Photoluminescence of Organic-Dye/TMD Hybrid Structures — •Julian Schröer, Lisa Böhme, Erik von der Oelsnitz, Alina Schubert, Rico Schwartz, Stefan Lochbrunner, and Tobias Korn — University of Rostock, Institute of Physics, AG Zweidimensionale Kristalle und Heterostrukturen

Thin layers of organic molecules and layered semiconductors build a new compound material with many interesting applications. The optoelectronic properties of these heterostructures strongly depend on the chosen compounds. In our work, we apply photoluminescence spectroscopy to hybrid structures of the organic dye perylene orange (PO) combined with monolayers of transition metal dichalcogenides (TMDs) like MoSe2, MoS2 and WSe2. These hybrid structures are candidates for fast and efficient charge or energy transfer due to their emerging type-II band alignment. Here, we aim to reveal the charge transfer processes in the different heterostructures by examining the excitation density-dependent low-temperature photoluminescence of the exciton and trion of the TMDs. Our work paves the way for a deeper understanding of organic/inorganic heterointerfaces and their application as photodetectors or light-harvesting devices.

HL 36.3 Wed 18:00 Poster E

Time-resolved Faraday ellipticity on multilayer WSe_2 — •Anna Weindl[1], Jennifer Lehner[1], Simon Raiber[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan

We report about our time-resolved Faraday ellipticity (TRFE) experiments on mulitlayers of the transition metal dichalcogenid WSe_2. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the temporal dynamics in WSe_2 multilayers. These previous results have shown that pseudospin oscillations appear in the TRFE signal when we apply an in-plane magnetic field to our samples. Now we try to characterize and manipulate these oscillations by playing with different experiment parameters. Varying the angle of the magnetic field, adding an electric field or investigating the layer dependence are examples for our toolbox of parameters to gain further insights in the dynamics of the multilayers.

[1] S. Raiber, P. E. Faria Junior, D. Falter, S. Feldl, P. Marzena, K. Watanabe, T. Taniguchi, J. Fabian, C. Schüller. Ultrafast pseudospin quantum beats in multilayer WSe_2 and $MoSe_2$, Nat. Commun. 13, 4997 (2022).

HL 36.4 Wed 18:00 Poster E

Giant band Splitting in WSe2/WTe2 heterostructure — •jiabao yang[1], wei yao[1], pavel dudin[2], jose avila[2], stuart parkin[1], and niels schröter[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg2, 06120 Halle(Saale), Germany — [2]Synchrotron SOLEIL, L*Orme des Merisiers , Saint Aubin BP 48, 91192 Gif sur Yvette Cedex, France

Two-dimensional (2D) heterostructures have emerged as a promising platform for investigating strongly correlated electronic phases. Transport measurements on WSe2/WTe2 have shown a switchable correlated insulating state by a ferroelectric field, but clearer evidence on how interlayer interaction and the formation of the Hubbard bands are influenced by ferroelectricity is still lacking. Based on Angle-Resolved Photoemission Spectroscopy (ARPES), we have found two interesting phenomena, the giant band splitting in the WSe2 layer with a ferroelectric WTe2 substrate, and the splitting of the bilayer WTe2 conduction band under the Moiré potential by WSe2.

HL 36.5 Wed 18:00 Poster E

Enhanced light-matter interaction in a monolayer of WS2 on top of Mie voids in a high-index material — •Padam Nagarkoti[1], Serkan Aslan[2], Hossein Ostovar[1], Mario Hentschel[2], Harald Giessen[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany

Light manipulation in subwavelength structures has gained significant attention in recent years. It is mostly based on the optical resonances in the metallic and dielectric materials. In this work, we numerically study the optical properties of Mie voids[1] created in the high index material using finite element method simulation. We calculate and visualize the electric field within the system, illuminating Mie voids from above. The simulation result shows that the light is entirely localized and confined within the void. Peaks in the reflectance spectra indicate resonant modes. We demonstrate that the resonance wavelength can be shifted by changing the dimensions of the void. Increasing either the height or diameter or both dimensions of the void, a red shift in the resonance wavelength is found. Furthermore, we show the coupling of resonant modes with WS2 monolayer on top of the void results in enhanced absorption. The absorption in the WS2 is optimized by tuning the void parameters. These results indicate that the 2D semiconducting materials in combination with Mie voids have a great potential for light trapping and solar energy conversion applications.[1] Hentschel et al. Light: Science & Applications (2023) 12:3

HL 36.6 Wed 18:00 Poster E

Optoelectronic Control of Interlayer Excitons in $MoSe_2/WSe_2$ Heterostructures — •Jan-Niklas Heidkamp[1], Johannes Krause[1], Swarup Deb[1], Takashi Taniguchi[2], Kenji Watanabe[2], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]National Institute for Material Science, Tsukuba, Japan

Transition-metal dichalcogenide (TMDC) heterostructures have recently garnered significant scientific interest due to their unique optical properties, including the emergence of tightly bound intralayer excitons and long-lived interlayer excitons. In this study, we investi-

gate the photoluminescence (PL) associated with interlayer excitons in heterostructures comprising molybdenum diselenide ($MoSe_2$) and tungsten diselenide (WSe_2). We aim to manipulate these quasiparticles using in-plane electric fields and modulation of the charge carrier density applied via microstructured electrodes and a potential difference across the heterostack. These experimental investigations provide valuable insights into the optical properties and behavior of interlayer excitons in TMDC heterostructures, offering prospects for their potential application in optoelectronic devices and photonics.

HL 36.7 Wed 18:00 Poster E

Amplification of interlayer exciton emission in twisted WSe2/WSe2/MoSe2 heterotrilayers — •Chirag Palekar[1], Paulo E. Faria Junior[2], Bárbara Rosa[1], Frederico Sousa[3], Leandro Malard[3], Jaroslav Fabian[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais 30123-970

Transition metal dichalcogenides (TMDC) heterostructures (HS) obtained by stacking two or more different monolayers (ML) host interlayer excitons (IX) with unique properties that depend on the twist angle and stacking order of MLs. However, IX*s practical applications are limited by the weak oscillator strength, leading a significant reduction in emission. Hence a viable path towards substantially improving the emission of IX is desirable. Here we investigate the twist angle dependent enhancement of IX emission in WSe2/WSe2/MoSe2 heterotrilayer (HTL) systems. The IX exciton formed in the HTL region exhibits a up to 10-fold increase in PL yield compared to HBL region on the same sample [1]. To understand the enhancement of the IX emission, we performed DFT calculations and effective modelling of the low energy IX states. This fundamental study of excitons in HTL system deepens the current understanding of twisted TMDC HSs and paves the way for further experiments, theoretical work and applications. [1] Palekar et al. arXiv:2311.02509,2023

HL 36.8 Wed 18:00 Poster E

Machine Learning based Monolayer Classification using a Convolutional Neural Network and Characterization of Transition Metal Dichalcogenides Heterostructures — •Maximilian Nagel, Chirag Palekar, Bárbara Rosa, Ching-Wen Shih, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

This research presents an advancement in the mass production of transition metal dichalcogenides (TMDCs) with potential benefits for the semiconductor industry. We introduce an automated system using convolutional neural networks (CNNs) for identification, classification and streamlining the monolayer search. Additionally, our study utilizes photoluminescence and second harmonic generation measurements for precise twist angle determination of heterostructures which are prepared using dry transfer method. By integrating data acquisition, image analysis, and machine learning, this innovative approach aids the TMDC heterostructure fabrication and enhances our understanding of TMDC heterostructures' properties. Collectively, this work represents a significant step forward in achieving cost-effective and efficient thin film manufacturing, with substantial implications for the semiconductor industry's future competitiveness and innovation.

HL 36.9 Wed 18:00 Poster E

Properties and Defects of hexagonal boron nitride grown by pulsed laser deposition — •Daniel Klenkert[1,2], Benedikt Winter[1], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University of Würzburg, 97074 Würzburg

Hexagonal boron nitride (hBN) has recently attracted significant research interest due to its unique properties. These include the chemical stability, its wide bandgap and the ability to host color centers inside the bandgap. These color centers exhibit bright and stable single photon emission at room temperature, which makes them interesting candidates for applications such as quantum communication and quantum sensing. To enable the direct pumping of color centers we examine the possibility to deposit hBN directly on LED and laser diode facets. As an intermediate step in this development, we report the results from spectroscopic measurements of hBN layers grown by pulsed laser deposition on silicon substrates as well as first tests on LEDs.

HL 36.10 Wed 18:00 Poster E

Enhanced room-temperature spin-valley coupling in Vanadium-doped MoS2 — •Krishna Rani Sahoo[1,2], Janmey Jay Panda[1], Sumit Bawari[1], Rahul Sharma[1], Dipak Maity[1], Ashique Lal[1], Raul Arenal[3], G Rajalaksmi[1], and Tharangattu N. Narayanan[1] — [1]Tata Institute of Fundamental Research-Hyderabad, Sy. No. 36/P, Gopanapally Village, Serilingampally Mandal, Hyderabad-500046, India — [2]Institute of Physics, University of Münster, Wilhelm-Klemm-Straße 10 48149 Münster, Germany — [3]Fundación ARAID, 50018 Zaragoza, Spain

Achieving room-temperature valley polarization in atomically thin materials by substitutional doping opens new avenues of spintronic applications. Here, we demonstrate that monolayer MoS2 (MS) doped with vanadium (V) at low concentrations exhibits high spin-valley coupling and hence a high degree of valley polarization at room temperature. A time-reversal symmetry broken energy shift in the equivalent valleys is predicted in V-doped MoS2 (VMS). Our room-temperature chirality-controlled photoluminescence excitation measurements indicate such a shift in valley exciton energies (~35 meV). An enhanced valley polarization in VMS (~42%) is observed in comparison to that in MS (<12%), while in MS, the chirality-controlled excitations did not show a difference in emission energies. Spin Hall effect of light-based optical rotation measurements indicate the asymmetric absorption among the two different chiralities of the incident light, hence supporting the existence of room-temperature valley polarization.

HL 36.11 Wed 18:00 Poster E

Optical characterization of non-magnetic 2D semiconductor MgPS3 and magnetic 2D semiconductor MnPS3 — •Thomas Kliewer[1], Pierre-Maurice Piel[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van-der-Waals (vdW) materials MnPS3 and MgPS3 are members of the metal phosphorus trichalgonides family (MPX3) which has recently gained interest due to its wide range of physical and chemical properties. MgPS3 is a possible photocatalyst for water-splitting reactions [1]. MnPS3 exhibits a ferromagnetic configuration between adjacent layers and an antiferromagnetic order in the layers [2] making it interesting for fundamental studies on magnetism in the 2D-limit.

Here we report on photoluminescence (PL)- and non-resonant Raman-spectroscopy investigations to characterize the optical and vibrational properties of both materials. To probe the impact of magnetic ordering, MnPS3 has been studied as function of temperature across the Néel-temperature.

For below-band gag excitation we find emission signatures in MnPS3 suggesting the existence of optically active in-gap states most likely due to defects. The Raman spectra of MnPS3 show the expected Raman active phonon modes. For MgPS3 the Raman-spectra show large intensity variations between different samples with different thickness.

[1] Jan Paštika et al. Small 18.18 (2022), p. 2200355 [2] Ko Kurosawa et al. J. Phys. Soc. Jpn. 52 (1983), pp. 3919-3926

HL 36.12 Wed 18:00 Poster E

Moiré Minibands, twist disorder and exciton-phonon coupling in van der Waals stacks — •Hendrik Lambers[1], Nihit Saigal[1], Nicolai-Leonic Bathen[1], Veljko Antic[1], Lennart Klebl[2], Dante M. Kennes[3], Tim O. Wehling[2], and Ursula Wurstbauer[1] — [1]University of Münster, Münster, Germany — [2]University of Hamburg, Hamburg, Germany — [3]RWTH Aachen University, Aachen, Germany

The weak van der Waals coupling between layers of most two-dimensional (2D) materials allows the realization of precisely tailored 2D quantum systems. Twisted homobilayers such as $tWSe_2$ are prone to the formation of moiré minibands. Guided by theoretical prediction, we study $tWSe_2$ homobilayer encapsulated in hBN by low-temperature resonant inelastic light scattering (RILS). We find resonant modes interpreted as single-particle collective inter-moiré-band excitations (IMBE) allowing to quantitatively probe the formation of a series of moiré-bands [1]. Moreover, we find that the resonance profiles particularly of the degenerated WSe_2 A_1'/E' phonon modes are significantly impacted by the assembly in vdW stacks suggesting a higher order Raman scattering process presumably involving simultaneous excitation and annihilation of phonon modes with finite momentum. [1] N. Saigal et al., arXiv:2310.14417 (2023).

HL 36.13 Wed 18:00 Poster E

Gas sensing of WSi_2N_4 in dark and bright environments — •Mustapha Driouech, Muhammad Sufyan Ramzan, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Two-dimensional materials are highly promising for gas sensing. In this work, we investigate the adsorption of the three common environmental gas molecules, namely O_2, CO_2, and H_2O on monolayer WSi_2N_4. Using density functional theory, we simulate molecular adsorption and evaluate resulting changes in the electronic structure of the monolayer in the dark and bright environment. The latter (former) is mimicked by promoting (removing) an electron to the conduction (valance) state. Our results show that all gas molecules are physically adsorbed on the WSi_2N_4 surface with small charge transfer in the dark. The presence of photogenerated electrons and holes changes the strength of gas adsorption. While with CO_2 and H_2O WSi_2N_4 behaves similarly in the dark and light environment, bright conditions enhance the interaction of WSi_2N_4 with O_2. As a result, charge transfer is increased compared to the dark, and substrate oxidation is promoted. Moreover, in terms of electronic properties, O_2 molecules contribute to the valence band maximum of the system regardless of the environment, making WSi_2N_4 a promising material for oxygen sensing.

HL 36.14 Wed 18:00 Poster E

Theory of Phonon Sidebands in the Absorption Spectra of Moiré Exciton-Polaritons — •Kevin Jürgens[1], Daniel Wigger[2], and Tilmann Kuhn[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany

Excitons in twisted bilayers of transition metal dichalcogenides experience a spatially varying electronic environment, which manifests in the formation of a periodic and twist-angle dependent moiré potential. For small twist angles the excitons are localized at the minima of the moiré potential, resulting in a flat band structure, whereas for large twist angles the excitons are almost entirely delocalized. When placing the heterostructure in an optical cavity, the moiré excitons interact with the photonic field, which leads to the formation of moiré exciton-polaritons. These couple to the lattice vibrations of the heterostructure giving rise to transitions between the two polariton branches that strongly depend on the twist angle.

We calculate the absorption spectra in the limit of small polariton densities. The polaritons are coupled to the same phonon bath, which results in inter- and intrabranch transitions in the polariton dispersion. We analyze the spectra and find rich phonon sidebands reflecting optical transitions assisted by phonon emission or absorption, that strongly depend on the twist angle. We identify the polariton gap and the presence of Van Hove singularities as critical parameters.

HL 36.15 Wed 18:00 Poster E

Investigating the Electrical Performance of Exfoliated Mono-Layer and Few-Layer Graphene — •Yasaman Jarrahi Zadeh, Felix Schaumburg, Jens Kerski, Günther Prinz, Martin Paul Geller, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

The groundbreaking discovery of two-dimensional (2D) graphene in 2004 sparked immense interest owing to its extraordinary electrical properties. Graphene's exceptional electron mobility makes it an ideal material for semiconductor devices that require fast response times. Additionally, the number of layers of graphene affects its different properties [1]. This study investigates the electrical behavior of exfoliated mono-layer and few-layer graphene structures on a Si substrate with SiO_2 top layer. To accomplish this, we employ the Van der Pauw method and Hall effect measurements to comprehend conductivity, carrier mobility, and quantum transport phenomena in both mono-layer and few-layer graphene. However, the characterization of ultrathin 2D material-based devices using electrical techniques poses challenges, and the conventional methods of characterization require optimization. By obtaining the electrical properties of graphene most optimally, further steps will be to enhance the performance of semiconductor devices like transistors and photodetectors.

[1] Urade, A.R., Lahiri, I. & Suresh, K.S. Graphene Properties, Synthesis and Applications: A Review. JOM 75, 614-630 (2023).

HL 36.16 Wed 18:00 Poster E

Nonlinear optical observation of time-reversal symmetry breaking in graphene — •Nele Tornow, Omid Ghaebi, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany

Monolayer graphene (MLG) provides the ideal platform to study the interplay between space inversion symmetry (IS), time-reversal symmetry (TRS), and topology [1]. The development of new ultrafast and non-perturbative all-optical spectroscopy methods could provide invaluable insights in this context, and nonlinear optics (NLO) is a promising approach thanks to its sensitivity to crystal symmetries.

In this work, we use NLO spectroscopy to investigate breaking of TRS in MLG, while preserving IS. To this end, we excite a MLG field-effect transistor with elliptically polarized light, i.e. with perfectly time and space superimposed and degenerate circular (pump) and linear (probe) beams. The circular pump breaks TRS, while the linear component probes the new terms generated in the NLO susceptibility, which result in a rotation of the emitted third-harmonic (TH) signal, in analogy with the valley nonlinear Kerr rotation observed in transition metal dichalcogenides [2]. Preliminary results further show a rotation of the TH signal as a function of both doping and excitation power.

Our results demonstrate a new method for all-optical generation and detection of broken TRS in MLG and thus a new powerful tool to explore topology in centro-symmetric crystals.

[1] McIver, J. W. et al., Nat. Phys. 16, 38-41 (2020)
[2] Herrmann, P. et al., Small 19, e2301126 (2023)

HL 36.17 Wed 18:00 Poster E

Optically gated acousto-electric effect in 2D semiconductors — •Felix Ehring, Benjamin Mayer, Clemens Strobl, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

With wavelengths in the micrometer range at GHz frequencies, surface acoustic waves (SAWs) are a versatile tool for radio frequency control and probing of charge carrier dynamics in novel semiconductor nanostructures. They are generated on a piezoelectric chip and routed over long distances to couple either mechanically or electrically with almost any nanosystems. In our experiments we fabricated hybrid lithium niobate SAW-devices including SAW delay lines with design frequencies of 150-250MHz containing gold electrodes on which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials can be placed. The dynamic electric field of the SAW induces a SAW power-dependent Acousto-Electric Current (AEC) in the different TMDC structures. The SAW directional dependence of this fundamental effect enables a detailed investigation of the TMDC interface.Through the spatially-resolved photodoping of the TMDC with a focused green laser (532nm), this setup can be utilized to study the charge carrier dynamics in a variety of different TMDCs, spanning from mono- to few-layer. [1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 36.18 Wed 18:00 Poster E

Pump-probe spectroscopy of Rydberg excitons in TMDC monolayers — •Max Wegerhoff, Moritz Scharfstädt, Andrea Bergschneider, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Quantum photonic technologies rely on strong optical nonlinearities, such as those provided by Rydberg atoms. The solid-state analog to this are Rydberg excitons. Rydberg excitons in cuprous oxides with principal quantum numbers of up to n=25 show strong optical nonlinearities, whose signatures could be detected by pump-probe spectroscopy [1]. In TMDC monolayers, which exhibit particularly strongly bound excitons, an increased nonlinearity could already be established for exciton-polaritons with n=2 [2].

Here, we report on the pump-probe spectroscopy of Rydberg states of excitons in TMDC monolayers at liquid helium temperatures. We use spectrally broad femtosecond probe pulses and a spectrometer to measure the transient differential reflectivity spectra. The degenerate pump-pulses are suppressed in a cross-polarized configuration such that the same Rydberg state is excited and probed. The doping of the monolayers is defined by electrical gating and kept neutral for the measurements.

[1] Heckötter, J., Walther, V., Scheel, S. et al., Nat Commun 12, 3556 (2021)
[2] Gu, J., Walther, V., Waldecker, L. et al., Nat Commun 12, 2269 (2021)

HL 36.19 Wed 18:00 Poster E

Photoluminescence emission of TMDC Monolayers under strain — •Pabin Rai, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Wilhelm-klemm-straße 10 48149 Münster Ger-

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Monolayers of transition metal dichalcogenides (TMDC) emit considerable photoluminescence despite their atomic thickness. The band gap of monolayers decreases when subjected to unidirectional mechanical tensile strain, resulting in a redshift in photoluminescence. Typically, uniaxial tensile strain is applied by bending a flexible polymer with a TMDC monolayer on top. However, this method causes strong sample displacement in the focusing direction, requires realignment after every strain step, and prevents the usage of high-numerical-aperture objective lenses. Here we demonstrate strain application by linearly pulling the flexible polymer substrate to circumvent these issues. These findings bear significance in advancing the development of strain-tuned optoelectronic devices.

HL 36.20 Wed 18:00 Poster E

Electrical transport properties of twisted bilayer graphene with twist angle disorder — •Bei Zheng, Xiaoyue Zhang, Fan Bai, Lina Bockhorn, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The twisting of the graphene layer opens up a whole new field of rich physics [1]. Especially, the electronic properties of twisted bilayer graphene depend strongly on the twist angle[2,3]. The twisted graphene structures around the magic angle were the first systems to show strong correlation behaviors, such as the rise of superconductivity and Mott's insulating phase [4,5].

We fabricated two twisted bilayer graphene samples around the magic angle via the "tear and stack" method. We investigated their transport properties by carrying out field effect measurements at different temperatures T from 300 K down to 1.4 K. The samples showed signatures of twist angle disorder and the resulting quantum interference. We analyzed the temperature- and carrier density-dependent conductance fluctuation ΔG_{xx} and concluded that, although the disorder of twist angle suppresses the superlattice effect and enhances the quantum interference, the coexistence of phase transition and quantum interference still can be observed since the phase-coherence length L_ϕ is one order of magnitude larger than the moiré superlattice constant λ_m for both samples. [1] H. Schmidt et al., Nat. Commun. 5, 5742 (2014) [2] J. C. Rode et al., 2D Mater. 3, 035005 (2016) [3] S. J. Hong et al., 2D Mater. 8, 045008 (2021) [4] Y. Cao et al., Nat. 556, 43-50 (2018) [5] X. Lu et al., Nat. 574, 653-657 (2019)

HL 36.21 Wed 18:00 Poster E

Anisotropic transport in 1D Bilayer Graphene Superlattices — •Julia Amann[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

One-dimensional superlattices (1DSLs) in graphene have been predicted to show intriguing effects, such as transport anisotropy, additional Dirac points and a distorted Fermi contour. In contrast to two-dimensional graphene superlattices, which have been widely studied, only very few experiments on 1DSLs have been reported. We use a patterned few-layer graphene gate underneath an encapsulated bilayer graphene to create a 1DSL. With the combined action of a global gate and a patterned bottom gate we can control superlattice potential strength and charge carrier density independently. We show low temperature transport measurements on a gate tunable 1DSL in bilayer graphene with a period of 50 nm in directions parallel and perpendicular to the modulation as we use a L-shaped Hallbar. We observe anisotropic transport in x and y directions and the appearance of multiple Dirac points in the modulation direction. These extra Dirac points are represented as additional Landau fans in magnetotransport. Furthermore, Weiss-oscillations are observed confirming the 1DSL modulation and the anisotropy.

HL 36.22 Wed 18:00 Poster E

Substitutional Doping of Exfoliated 2D Materials — •Sirri Batuhan Kalkan[1], Felix Junge[2], Hans Hofsäss[2], and Thomas Weitz[1] — [1]I. Institute of Physics, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]II. Institute of Physics, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Low-energy (<50 eV) ion implantation is a versatile technique for creating novel two-dimensional electronic devices by doping with electrons, holes, or inducing magnetism [1-3]. These modified films can be utilized as electrodes in energy-efficient electrochemical processes, homojunctions of the same material, or unique spintronic devices. In this poster, we discuss the optimization of the implantation processes for mechanically exfoliated 2D materials. We cover several topics, including improvements through post-cleaning approaches, the influence of doping-induced defects, the fabrication of prototype van der Waals heterostructure devices, and their characterization.

References: [1] Willke, Philip, et al. "Doping of graphene by low-energy ion beam implantation: structural, electronic, and transport properties." Nano Letters 15.8 (2015): 5110-5115 [2] Lin, Pin-Cheng, et al. "Doping graphene with substitutional Mn." ACS nano 15.3 (2021): 5449-5458. [3] Pramanik, Arindam, et al. "Anomalies at the Dirac Point in Graphene and Its Hole-Doped Compositions." Physical Review Letters 128.16 (2022): 166401

HL 36.23 Wed 18:00 Poster E

Wavelength-Dependent Optical Excitation and Depth-Resolved Photoluminescence Spectroscopy of Defects in hexagonal Boron Nitride — •Diana Gühring[1], Paul Konrad[1], Lina M. Todenhagen[2], Andreas Sperlich[1], Igor Aharonovich[3], Martin S. Brandt[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [2]Walter Schottky Institute and School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

In recent years, quantum emitters in 2D materials, such as hexagonal Boron Nitride (hBN), have shown promising applications in various fields of quantum technology. Although the recently discovered boron vacancy ($V_B{}^-$) spin-defect center in hBN is especially promising for nanoscale sensing, a deeper insight into its optical properties remains unexplored. Here, the wavelength-dependent optical excitation in correlation with photoluminescence (PL) is investigated to gain insights into the fundamental characteristics of $V_B{}^-$. Furthermore, the study includes confocally resolved, depth-dependent PL spectroscopy, examining the impact of the environment on the observed PL. The findings presented here contribute to a comprehensive understanding of the optical properties of defects in hBN, offering valuable insights for an efficient exploitation of this promising quantum material.

HL 36.24 Wed 18:00 Poster E

Towards magnetotransport measurements in rhombohedral penta-layer graphene — •David Urbaniak, Christian Eckel, Anna Seiler, and Thomas Weitz — University of Göttingen, Faculty of Physics, 1st Institute of Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Graphene is one of the most studied 2D material to-date. Due to its band structure, rhombohedrally stacked multi-layer graphene has been the subject of recent studies. Notably the discovery of superconductivity in tri-layer graphene attracted significant attention [1]. Penta-layer graphene is currently of particular interest for the study of electron correlation effects due to its high density of state stemming from increased flat bands near the band edge [2, 3]. This work shows how rhombohedrally stacked regions of mechanically exfoliated penta-layer graphene can be identified via Raman spectroscopy and spatially resolved in the nanometer regime by scanning near field optical microscopy (SNOM). Furthermore, a nanolithography technique to isolate such regions using an atomic force microscope (AFM) is presented, as well as the fabrication steps of hexagonal Boron Nitride (hBN) encapsulated dual gated magnetotransport devices and the stability of the rhombohedral stacking order during the fabrication process. Additionally, an outlook on the upcoming magnetotransport measurements in the milli Kelvin regime is discussed.

References: [1] Zhou, Haoxin, et al. Nature 598.7881 (2021): 434-438. [2] Han, Tonghang, et al. Nature 623, 41-47 (2023) [3] Han, Tonghang. et al. Nat. Nanotechnol. (2023)

HL 36.25 Wed 18:00 Poster E

Multi-method characterization of initial growth of a MoS_2 layer by atomic layer deposition — •Christian Petersen, Christian Tessarek, Alexander Karg, Alexander Hinz, Niels Osterloh, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

MoS_2 is a 2D semiconductor with exceptional optical and electrical properties, thus considered as a possible future material for ultra-thin film transistors or optoelectronic devices. To overcome size limitations due to exfoliation, synthesis methods like chemical vapour deposition or atomic layer deposition (ALD) bear the possibility for large scale controlled fabrication of pristine monolayers.

In this comprehensive study MoS_2 layers grown by ALD from submonolayer to the bilayer regime are analyzed. The surface morphology was investigated by atomic force microscopy (AFM). In addition, X-ray photoelectron spectroscopy (XPS) was used for a chemical analysis while Raman as well as photoluminescence (PL) spectroscopy revealed structural and optical properties. In combination of these methods the monolayer growth regime was identified and a growth model is proposed that is used explain the obtained results.

HL 36.26 Wed 18:00 Poster E

Resonant and non-Resonant Raman spectroscopy on the magnetic semiconductor CrSBr — •Oskar Schröer[1], Pierre-Maurice Piel[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

CrSBr, a van der Waals (vdW) material, exhibits a remarkable combination of attributes. It is an optically active, air-stable magnetic semiconductor, and its vdW structure endows it with magnetic properties characterized by ferromagnetic ordering within each layer and antiferromagnetic coupling between adjacent layers. This unique electronic band structure imparts strong anisotropy, effectively transforming the material into a quasi-one-dimensional system [1]. As a result, CrSBr's direct band gap is marked by robust, anisotropic excitonic resonances, rendering it particularly intriguing to study interaction physics. For opto-spintronic applications, it is imperative to cultivate a profound understanding of its quasi-particles, their interactions, and their intricate interplay with magnetic order. Here, we report on temperature dependent photoluminescence (PL) as well as resonant and non-resonant Raman spectroscopy experiments below and above the Néel temperature to study the impact of the magnetic ordering in bulk CrSBr. We find that peculiar signatures only observable in resonant Raman spectra are indicative for the magnetic phase transition from the anti-ferromagnetic to the paramagnetic state. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023)

HL 36.27 Wed 18:00 Poster E

Interlayer excitons engineering in Transition Metal Dichalcogenides Heterobilayer — •Ridha Eddhib, Aki Pulkkinen, and Jan Minar — New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic.

Our study is aimed to showcase the feasibility of manipulating the optical characteristics of transition metal dichalcogenide Heterostructures (TMD-HS) beyond the intralayer excitons[1-2], particularly when one of the constituent layers adopts a ternary structure which is an intriguing class of HS known as type II band alignment. This manipulation bears crucial implications for enhancing charge separation efficiency, as optically excited electrons and holes undergo relaxation into distinct material layers giving rise to interlayer excitons. In the realm of binary-ternary (B-T) HS systems, we have investigated the exciting avenue for extending the energy range and tailoring emission energies, surpassing the capabilities of their (B-B) and free standing counterparts. Our findings underscore the significance of the alloying ratio in fine-tuning excitons binding energy, and also highlighting the importance in the band offset in the emergence of this optical feature thereby introducing a novel design parameter for tailoring optoelectronic devices to specific applications. [1] Hichri, A., T. Amand, and S. Jaziri. Physical Review Materials 5.11 (2021): 114002. [2]Aly, M. A., Enakerakpor, E. O., Koch, M., & Masenda, H. (2023). Nanomaterials, 13(20), 2769.

HL 36.28 Wed 18:00 Poster E

Ion-irradiated hBN-silicon hybrid photodetectors for near infrared polarized imaging — •Peiting Wen[1,2], Mohd Saif Shaikh[1,2], Jiang Qu[3], Shuyu Wen[1], Ye Yuan[4], Slawomir Prucnal[1], Manfred Helm[1,2], Artur Erbe[1,2], Shengqiang Zhou[1], and Yonder Berencén[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01062, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, 01069, Germany — [4]Songshan Lake Materials Laboratory, Dongguan, Guangdong, 523808 China

Beyond being an excellent encapsulant and gate dielectric 2D material, hexagonal boron nitride (hBN) is significant in exploring the use for polarized photonics functionalities. Optically active defects in the h-BN are intriguing, serving not only to enable the optical readout of spins but also to function as quantum emitters that operate at room temperature. Furthermore, the creation of defects in hBN disrupts the symmetry of the lattice and induces an in-plane anisotropic crystal structure. Here, we will uncover intriguing in-plane anisotropic phenomena in Raman response and photoluminescence in 2D hBN subjected to ion irradiation. Leveraging this discovery, we seamlessly integrated the ion-irradiated hBN into room-temperature p-i-n Si detectors. Notably, the ion-irradiated hBN will serve as the polarized-sensitive layer, while Te hyperdoped silicon will facilitate infrared absorption. This hybrid structure highlights its potential as a polarized sensitive photodetector for the applications of image sensing and the ability of compatible with the CMOS process.

HL 36.29 Wed 18:00 Poster E

Proximity-induced exchange field in a 2D magnet/graphene heterostructure detected by the anomalous Hall effect — Maximilian Luka[1], •Stefan Peterhans[1], Matthias Kronseder[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Since the first observation of magnetic order in 2D materials in 2017, several groups have exploited the properties of these materials, opening up a new field in addition to the vast range of 2D crystals. Materials such as, e.g., $Cr_2Ge_2Te_6$ (CGT) can be used to induce magnetic properties in single or bilayer graphene due to the magnetic proximity effect. These magnetic exchange fields can be detected by measuring the anomalous Hall effect (AHE). We were able to observe the AHE in a graphene/CGT/hBN-heterostructure. This observation was supported by SQUID-measurements to show the temperature dependence of the magnetization of CGT and its effect on the strength of the AHE. To exclude a trivial stray field effect, we measured the magnetic stray field of several magnetic materials (Fe_3GeTe_2, CGT) with graphene Hall micromagnetometry, where the 2D magnet was not in direct contact with the graphene layer. The signal detected in this configuration was significantly weaker than the AHE in the proximity-coupled heterostructure, confirming the presence of a magnetic proximity effect.

HL 36.30 Wed 18:00 Poster E

Exciton condensation in $TiSe_2$ detected by screening of single-layer WSe_2 — •Adrian Dewambrechies, Benjamin Weintrub, and Kirill Bolotin — Freie Universität Berlin, Germany

Two-dimensional materials and the recent progress in their manipulation have provided a platform to study highly correlated phenomena, a relevant case being the condensation of the excitons dominating their optical response. Recent advances show that the exciton properties, and their tunability in such systems, offer the observation of high temperature condensation, and allows the study of the crossover between different types of condensates including the Excitonic Insulator. However, a definitive proof of the exciton condensation and superfluidity is still missing mainly due to the charge of excitons being zero, and new experimental techniques are being explored in this direction. Here, we present our latest results in the detection of exciton condensation in two-dimentional semimetal $TiSe_2$. We study its effect in the dielectric environment of a nearby sensor layer of WSe_2, by tracking the emission and absorption of its excitons to understand charge transfer between the two materials and the potential transition to an excitonic insulating state in $TiSe_2$.

HL 36.31 Wed 18:00 Poster E

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

Among two dimensional semiconductor materials, transition metal dichalcogenides (TMDCs), such as molybdenum disulfide, are studied the most. More recently, 2D Janus materials based on TMDCs were discovered. They can be created by exchanging one of the chalcogen layers in a base TMDC with another species of chalcogen atoms, thus forming an asymmetrical Janus structure with new, unique properties [1]. As the process selectively substitutes the top-most layer of chalcogen atoms with another kind, there is a likelihood of a partial substitution. In such instances the resulting material would resemble an alloy more closely than a Janus structure. These alloys consist of regions with different stoichiometry, which means they represent an ideal bridge between the characteristics of the base TMDC and the ideal Janus materials.

With my poster, I will showcase my latest achievements in synthesizing Janus materials and their alloys, and the characterization of their features with Raman and Photoluminescence spectroscopy.

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

HL 36.32 Wed 18:00 Poster E

Light induced dynamics in a coupled van der Waals heterostructure — •Mashood Tariq Mir, Arne Ungeheuer, Ahmed Hassanien, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

Layered transition metal dichalcogenides (TMDs) host a rich collection of physical properties, opening many applications with atomically thin films such as sensors, electronic switching, or energy storage. Among those materials, 1T-TaS2 exhibits a complex phase diagram depending on temperature encompassing charge density waves (CDW) with diverse commensurabilities. New phenomena have been observed and are further expected from combining different materials to 2D heterojunctions. We employ the UED technique to investigate the light-induced dynamics in the sub-ps time regime. This work uses femtosecond laser pulses to induce rapid structural changes in a free-standing van der Waals heterostructure. Upon lattice heating, the CDW material undergoes several phase transitions. We focus on the reversible phase transition 1T-TaS2 from the nearly commensurate to the incommensurate phase. In addition, we present an initial UED study on the optically excited CAPs in a stacked (1T-TaS2 / Graphite) heterostructure.

HL 36.33 Wed 18:00 Poster E

Coherent interlayer phonons in van der Waals MoSe2/WSe2 heterobilayers — Changxiu Li[1,2], Alexey V. Scherbakov[1], •Pedro Soubelet[3], Anton K. Samusev[1], Claudia Ruppert[1], Nilanthy Balakrishnan[4], Vitalyi E. Gusev[2], Andreas V. Stier[3], Jonathan J. Finley[3], Manfred Bayer[1], and Andrey V. Akimov[5] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Germany. — [2]Laboratoire d'Acoustique de l'Université du Mans, Institut d'Acoustique-Graduate School, Le Mans Université, France. — [3]Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Germany. — [4]School of Chemical and Physical Sciences, Keele University, United Kingdom. — [5]School of Physics and Astronomy, University of Nottingham, United Kingdom.

The increasing role of two-dimensional (2D) devices requires the development of new techniques for ultrafast control. A special feature of heterobilayers (HBs) assembled from van der Waals (vdW) monolayers is the femtosecond separation of photoexcited electrons and holes between the neighboring layers, resulting in the formation of Coulomb forces. Using laser pulses, we generate a 0.8THz coherent breathing mode in MoSe2/WSe2 HBs, which modulates the thickness of the HB and should modulate the photogenerated electric field in the vdW gap. While the phonon frequency and decay time are independent of the stacking angle between monolayers, the amplitude decreases at intermediate angles, which is explained by a decrease in the photogenerated electric field between the layers.

HL 36.34 Wed 18:00 Poster E

Layered Minerals and Chalcogenides investigated by Atom Probe Tomography — •Jan Köttgen[1], Alexander Kiehn[2], Anna Vymazalová[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]1. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Institute "Green IT (PGI-10)", Forschungszentrum Jülich, 52428 Jülich, Germany — [3]Czech Geological Survey, Geologická 6, 152 00, Prague, Czech Republic

Layered solids have recently attracted considerable attention due to the vast range of properties that can be realized in such layered systems. Layered chalcogenide compounds, in particular, exhibit a rich variety of structures. Some of these materials also employ metavalent bonding, which is a distinctive bonding mechanism initially discovered in crystalline phase change materials (PCM). The bonding between the atoms can be investigated by breaking these bonds in atom probe tomography. Compounds such as GeTe or Sb_2Te_3 exhibit unconventional properties indicative for the presence of metavalent bonding e.g. typically one electron per bond shared between atoms, and a high probability of multiple events observed in atom probe tomography. The aim of this project is to better understand the relation between layered solids and metavalent bonding, focusing on the transition metal chalcogenides $PdTe_2$ and Pt_3Te_4, and comparing them with layered minerals like vihorlatite ($Bi_{24}Se_{17}Te_4$). All layered systems investigated exhibit a high multiplicity during laser-assisted atom probe tomography, indicative for an unusual bonding mechanism. Further experiments will be presented which help to classify and understand these layered solids.

HL 36.35 Wed 18:00 Poster E

Size Dependence of Electrical Properties of Thin Film $ZrSe_3$ — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Among the popular group of transition metal chalcogenides, the transition metal trichalcogenides show unique properties, such as a quasi-1D structure [1]. Previous work displayed different electrical properties of $ZrSe_3$ [2]. Building on this, the influence of the sample geometry on the electrical properties of thin film $ZrSe_3$ was investigated. The bulk material used was fabricated by a chemical vapor transport method and then exfoliated to achieve thin films.

We determined band gap energies for samples with varying heights. Those are shown to increase linearly from 0.37 eV to 0.63 eV as the thickness of the material decreases from 35 nm to 14 nm. Furthermore, an unusual width dependence of the conductivity in thin $ZrSe_3$ was found. By comparing the widths and conductivities of wide and narrow samples, a non-linear increase in the conductivity ratio with increasing width ratio was observed.

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

HL 36.36 Wed 18:00 Poster E

Realizing thermoelectric transport measurements in dual-gated Bernal bilayer graphene — •Moritz Knaak, Martin Statz, and Thomas Weitz — University of Göttingen, Faculty of Physics, 1st Institute of Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In dual-gated, hexagonal boron nitride (hBN) encapsulated, trigonally warped Bernal bilayer graphene (BLG) many correlated phases at high out-of-plane electric fields have been found.[1-3]. They were found close to Lifshitz transitions, where the density of states(DoS) is high and which can be induced by tuning the out-of plane electric field or the charge carrier density. While conductance measurements alone only give an indirect probe of the DoS, in thermoelectric transport measurements we can study the Seebeck coefficient, which provides a more direct probe of it. To measure the Seebeck coefficient, we use an on-chip heater next to the hBN-encapsulated BLG which is dual-gated and contacted by graphite gates and contacts. The source-drain contacts are simultaneously used as 4-point-probe on-chip resistance thermometers to determine the local temperature differences. A dry-transfer method, e-beam-lithography, reactive ion etching as well as thermal evaporation of contact leads are employed for the fabrication of the thermoelectric devices.

[1] Seiler, A.M. et al. Nature 608, 298-302 (2022) [2] Zhou, H. et al. Science 375, 774-778 (2022) [3] de la Barrera, S. C. et al. Nat. Phys. 18, 771-775 (2022)

HL 36.37 Wed 18:00 Poster E

Optical spectroscopy of atomically thin MoS_2 under high pressure — •Paul Steeger, Jan-Hauke Graalmann, Robert Schmidt, Philipp Marauhn, Marie-Christin Heissenbüttel, Jan Nellesen, Ilya Kupenko, Carmen Sanchez-Valle, Steffen Michaelis de Vasconcellos, Miachel Rohlfing, and Rudolf Bratschitsch — University of Münster, Germany

High-pressure diamond anvil cells (DACs) are a recent addition to the toolkit for investigating two-dimensional materials and their heterostructures. They can exert compressive strain to samples, allowing precise manipulation of interlayer coupling strength in multi-layered van der Waals materials. Here, we present pressure-dependent optical transmission spectra of 2H-MoS_2 bilayers under pressure and extract the respective energy shift rates of inter- and intralayer excitons. Additionally, our findings highlight an interesting observation: the actual deformation of the sample differs from hydrostatic compression due to substrate effects. We discuss strategies to address this common challenge encountered in high-pressure experiments on 2D materials in conjunction with complementary DFT-based calculations. [1]

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

HL 36.38 Wed 18:00 Poster E

Cryogenic nano-imaging of the metal to charge density wave transition in NbSe2 — •Monica Kolek Martinez de Azagra, Francesca Falorsi, Christian Eckel, and Thomas Weitz —

Georg-August-Universität Göttingen

The transition metal dichalcogenide (TMDC) NbSe2 exhibits a metallic, charge density wave (CDW) - the periodic modulation of electron densities and lattice atoms - and a superconducting phase. The transition between these phases can be tuned by temperature variation. Previous studies have shown that the critical temperatures TCDW for the CDW transition and TC for the superconductivity are layer dependent. While calculations have shown that with decreasing layer thickness the CDW order is enhanced with a gain in energy [1], experimental results contradict each other regarding the TCDW for few-layer and bulk NbSe2. [2,3] Here, we present our preliminary results on the investigation of 2H-NbSe2 using a cryogenic scanning near-field microscope (SNOM), to image the layer-dependent TCDW. Using SNOM we are able to provide real-space images while probing the dielectric function of the NbSe2 few-layer flakes with nanometer resolution. Subsequently, we will be able to verify our results using transport measurements in situ.

HL 36.39 Wed 18:00 Poster E

Optimization of magnetic topological insulators by magneto-transport measurements — •Jonas Buchhorn[1,2], Jan Karthein[1,2], Kaycee Underwood[1,2], Abdur Rehman Jalil[1,2], Michael Schleenvoigt[1,2], Peter Schüffelgen[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich und RWTH Aachen University, 52425 Jülich, Germany

Edge channels in magnetic topological insulators in the quantum anomalous Hall state are a promising platform for quantum computing, when they are in proximity to a superconductor. Majorana modes are proposed to emerge which by non-abelian braiding statistics lead to a fault-tolerant computing paradigm. In this work, probing the chiral edge channels in Cr-doped $(Bi_xSb_{1-x})_2Te_3$ thin films is shown together with other properties of this material system that are observable by quasi DC magneto-transport measurements in Hall bars at cryogenic temperatures. A time-efficient feedback loop between electrical measurements and molecular beam epitaxy was established to investigate the impact of growth parameters on the magneto-transport properties of the thin films with minimal fabrication. The results of the feedback loop are presented and, together with the findings of the Hall bar measurements, they lead to a guideline on how to tune the magnetic topological insulator into the bulk- and surface-insulating regime, isolating the chiral edge channels from residual conductance.

HL 36.40 Wed 18:00 Poster E

Efforts to make Josephson junction on a quantum anomalous Hall insulator — •Bibek Bhujel[1], Anjana Uday[1], Gertjan Lippertz[1,2], Kristof Moors[3], Henry F. Legg[4], Andrea Bliesener[1], Lino M. C. Pereira[2], Alexey A. Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany — [2]KU Leuven, Quantum Solid State Physics, Celestijnenlaan 200 D, 3001 Leuven, Belgium — [3]Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, 52425 Jülich, Germany — [4]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Recently, we obtained evidence for superconducting pair correlation in the chiral edge states of a vanadium-doped $(Bi_xSb_{1-x})_2Te_3$ thin film that is tuned to the quantum anomalous Hall insulator phase, by observing the negative nonlocal resistance downstream from a narrow superconducting (grounded) Nb finger electrode [1]. This negative downstream resistance is due to the crossed Andreev reflection (CAR) process, which creates superconducting correlations in the chiral edge. To further investigate the superconducting proximity effect, we are currently fabricating Josephson junction on QAHI. This is a difficult experiment because the 2D "bulk" of the QAHI is insulating and the ferromagnetism works against superconductivity. We will report the progress we have made so far by using Nb electrodes.

[1] A. Uday et al., arXiv:2307.14196

HL 36.41 Wed 18:00 Poster E

Thermal anisotropy of $\beta - Ga_2O_3$ on ultra-short length scales — Moritz Meissner[1], •Luca Sung-Min Choi[1], Alwin Wüthrich[1], Kai Xu[2], Riccardo Mincigrucci[3], Laura Foglia[3], Danny Fainozzi[3], Filippo Bencivenga[3], Sebastian Reparaz[2], and Markus R. Wagner[1,4] — [1]Technische Universität Berlin, Berlin, Germany — [2]Institut de Ciència de Materials de Barcelona, Barcelona, Spain — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The monoclinic beta-phase of gallium oxide, known for its ultra-wide bandgap, emerges as a promising candidate for power electronic device technologies. We examine whether the macroscopic thermal anisotropy persists on the nanoscale. Employing the optical transient thermal grating (TTG) method, we determine the in-plane anisotropy of thermal transport and acoustic phonons across different grating length scales ranging from 110 to 26 nm. Thereby examining potential length-scale dependencies of the $\beta - Ga_2O_3$ anisotropy. Our experiments, conducted at the Fermi Free Electron Laser (FEL) [Elettra Synchrotron Trieste, dedicated endstation EIS-TIMER] on a (001)-$\beta - Ga_2O_3$ sample, enable the observation of thermal effects at ultra-short length scales.

HL 36.42 Wed 18:00 Poster E

Thermal Conductivities of Crystalline Polymers calculated with Machine-Learned Potentials — •Lukas Reicht, Lukas Legenstein, Sandro Wieser, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Disordered polymers are typically characterized by a very low thermal conductivity on the order of 0.1 W/mK. In contrast, recent experiments showed that, when polymers are highly aligned (crystalline), polyethylene (PE) can reach a thermal conductivity of ˜104 W/mK, which would be interesting for applications. Newly developed machine-learned potentials (MLP) promise to be an efficient and accurate tool for calculating these thermal conductivities. Applying a new methodology, however, requires a thorough benchmarking. We performed such a benchmarking for moment tensor potentials (MTPs), which are a flavour of machine-learned potential, by calculating various phonon related properties of polyethylene (PE), polythiophene (PT), and poly(3-hexyl-thiophene) (P3HT). Based on the calculated phonon band-structures, elastic constants, thermal expansion coefficients, and thermal conductivities, we conclude that the accuracy of MTPs can be substantially increased by a deliberate choice of training data adapted to the intended use case. Having established the accuracy of the trained MTPs, they are used to calculate thermal conductivities of PE and PT using the Boltzmann transport equation (BTE), non-equilibrium molecular dynamics (NEMD), and the approach-to-equilibrium molecular dynamics (AEMD). This provides complementary atomistic insights into the factors determining heat transport.

HL 36.43 Wed 18:00 Poster E

Phonon Bands and Thermal Conductivities of Organic Semiconductors using Machine-Learned Moment Tensor Potentials — •Lukas Legenstein[1], Lukas Reicht[1], Sandro Wieser[1], Michele Simoncelli[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]TCM Group, Cavendish Laboratory, University of Cambridge, UK

Phonons affect transport properties in crystalline organic semiconductors either by scattering with charge carriers, or as the main carriers of thermal energy. Modelling these phonons and their transport gives a distinct advantage of providing direct insight into the relevant processes at an atomistic level compared to experiments. Of particular relevance for such simulations are machine-learned potentials, which often achieve accuracies comparable to the ab initio methods they are trained on, albeit at hugely reduced computational costs. In this work we use Moment Tensor Potentials (MTP) to determine the phonon properties of the acenes (from benzene to pentacene). We show that the MTPs excellently reproduce the phonon bands calculated previously using dispersion-corrected density-functional theory. Further, we determine the lattice thermal conductivity by solving the Wigner transport equation. With this methodology the conduction mechanisms arising from inter-band tunneling are accounted, which turns out to be crucial for matching the temperature-dependent experimental values for naphthalene and anthracene. Importantly, the presented approach provides direct insight into the (anisotropic) contributions of individual modes to the thermal conductivities.

HL 36.44 Wed 18:00 Poster E

Nitrogen-doped Ni-TiO2 Nanoarrays via plasma treatment as Sodium-Ion Battery Anodes — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-ion batteries (SIBs) are a potential substitute for Li-ion batteries for energy storage devices due to their abundant reserves and low sodium cost. TiO2 is considered one of the promising anodes for SIBs due to its large sodium storage capacity. However, low electrical conductivity greatly reduces its rate performance and limits the broad application of TiO2 for SIBs. Here, we fabricated 3D Ni-TiO2 core-shell nanoarrays using nanoimprinted AAO templating and atomic layer deposition (ALD) technique. Then, the 3D Ni-TiO2 nanoarrays were treated via a nitrogen plasma system and directly used as anode. The 3D Ni-TiO2 arrayed anode can offer fast electron transport and high ion accessibility, and the nitrogen-doping also significantly improves the electrical conductivity of TiO2, resulting in a significant enhancement of the electrochemical performance, especially the rate performance.

HL 36.45 Wed 18:00 Poster E

Energy landscape around the $B_{Si}Si_i$ defect - a DFT Study — •Aaron Flötotto[1], Wichard J. D. Beenken[1], Kevin Lauer[1,2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is an important dopant of silicon. It often forms the so-called $B_{Si}Si_i$ defect, which has been suggested as a source of light-induced degradation (LiD) in solar cells made from boron-doped Czochralski-grown silicon [1]. In this study, we calculated the energy landscape around the $B_{Si}Si_i$ defect by first principle methods. This includes also configurations with only one interstitial B atom as well as a B–Si pair sharing a vacancy in the lattice. Between the meta-stable defect configurations we identified minimal energy paths utilizing the Nudged Elastic Band method. The resulting potential energy landscape is compared with previous models for boron diffusion and LiD. For the latter we identified possible recombination centers among the meta-stable defect configurations by their electronic DOS.

HL 36.46 Wed 18:00 Poster E

High-performance aqueous zinc-ion batteries based on the three dimensional manganese vanadate nanoflower cathode — •Yan Ran[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

In this work,manganese vanadate(MnVO) synthesized via a one-step hydrothermal method is proposed as a promising cathode material for AZIBs. Because the stable layered structure and hieratical morphology of MnVO provide a large layer space for rapid ion transports, this material exhibits high specific capacity (433 mAh g-1 at 0.1 A g-1), an outstanding long-term cyclability (5000 cycles at a current density of 3 A g-1), and an excellent energy density. To illustrate the intercalation mechanism, ex situ X-Ray diffraction, Fourier transform infrared spectroscopy, and X-ray photo-electron spectroscopy are adopted, uncovering an H+/Zn2+ dual-cation co-intercalation processes. In addition, density-functional theory calculation analysis shows that MnVO has a delocalized electron cloud and the diffusion energy barrier of Zn2+ in MnVO is low, which promotes the Zn2+ transport and consequently improves the reversibility of the battery upon deep cycling. The key and enlightening insights are provided in the results for designing high-performance vanadium-oxide-based cathode materials for aqueous zinc ion batteries.

HL 36.47 Wed 18:00 Poster E

High-performance aqueous zinc-ion batteries based on the three dimensional manganese vanadate nanoflower cathode — •Yan Ran[1], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

In this work, manganese vanadate (MnVO) synthesized via a one-step hydrothermal method is proposed as a promising cathode material for aqueous zinc ion batteries (AZIBs). Because the stable layered structure and hieratical morphology of MnVO provide a large layer space for rapid ion transports, this material exhibits high specific capacity (433 mAh g-1 at 0.1 A g-1), an outstanding long-term cyclability (5000 cycles at a current density of 3 A g-1), and an excellent energy density. To illustrate the intercalation mechanism, ex situ X-Ray diffraction, Fourier transform infrared spectroscopy, and X-ray photo-electron spectroscopy are adopted, uncovering an H+/Zn2+ dual-cation co-intercalation processes. In addition, density-functional theory calculation analysis shows that MnVO has a delocalized electron cloud and the diffusion energy barrier of Zn2+ in MnVO is low, which promotes the Zn2+ transport and consequently improves the reversibility of the battery upon deep cycling. The key and enlightening insights are provided in the results for designing highperformance vanadium-oxide-based cathode materials for AZIBs.

HL 36.48 Wed 18:00 Poster E

Structural reconfiguration of Bi(111) thin layers upon Na intercalation — •Peter Markmann, Uwe Gerstmann, Wolf Gero Schmidt, Guido Grundmeier, and Adriana Bocchini — Paderborn University, Warbuger Str. 100, 33098 Paderborn

Current technologies for energy storage are mainly based on lithium-ion batteries. Due to the low abundance of Li in the earth crust, other elements, e.g. heaviear alkali ions like sodium have to be considered for near future technology, but require well-adapted material for the electrodes.

In this work, with the help of DFT calculations, we investigate Bi(111) thin layers as a possible candidate. We show that the material in fact allows for interacalation of Na atoms in high concentrations up to 50 %, whereby the volume expansion is moderate and limited to the direction perpendicular to the Bi bilayers. Interestingly, if local concentration reaches atomic ratios of 1:2, a structural reconfiguration takes place, characterized by the appearance of 35°-tilted fractions of Bi-bilayers. Notably and in contrast to oxidization, this structural phase transitions is fully reversible under Na deintercalation and further reduces the volume expansion.

HL 36.49 Wed 18:00 Poster E

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HL 36.50 Wed 18:00 Poster E

Accurate computational description of electronic and structural properties of bismuth vanadate — •Philip Schwinghammer, Frederico Delgado, Franziska Hegner, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The electronic and structural properties of bismuth vanadate (BVO) were characterized using density functional theory (DFT). Previous work in the literature indicated that semi-local density functionals did not correctly reproduce the ground state geometry but disagreed on which functional would improve the description. We found that the Heyd-Scuseria-Ernzerhof hybrid functional could accurately predict the monoclinic ground state structure, provided spin-orbit coupling was included. Semi-local density functionals mischaracterize the hybridization of the lone pair Bi6s states and O2p states near the valence band edge, which is corrected by hybrid functionals. In addition, we also found the electronic properties to depend significantly on the inclusion of spin-orbit coupling. Particularly the states near the valence band edge have a profound impact on the monoclinic distortion, indicating that a reliable description of BVO is only possible when fully accounting for the relativistic effects due the heavy bismuth ions and using hybrid functionals.

HL 36.51 Wed 18:00 Poster E

Electrochemical properties of F-doped $RbTiOPO_4$ (RTP:F) predicted from first principles — •Yingjie Xie, Uwe Gerst-

mann, Wolf Gero Schmidt, and Adriana Bocchini — Universität Paderborn, 33095 Paderborn, Germany

Battery technologies based on heavier alkali ions are considered promising candidates to substitute for current Li-based technologies. However, due to the larger ionic radii, new electrode materials are required to guarantee, e.g., high energy densities, a fast ion (de)intercalation, and a robust long-term operation. In this context, many recent studies suggest the potassium titanyl phosphate ($KTiOPO_4$, KTP) crystals as promising electrodes in alkali-ion batteries [1-4].

Here, we characterize the structural properties of a novel KTP-type material, i.e., $RbTiPO_4F$ (RTP:F), and discuss its electrochemical performance for Rb-ion batteries (RIBs) using density functional theory (DFT). The material shows promising electrochemical properties for cathode application: A rather high average voltages of more than 2.8 V and a modest volume shrinkage of less than 13% are predicted upon the deintercalation of Rb.

[1] Fedotov et al., Chem. Mater. 26, 411 (2016)
[2] Fedotov et al., J. Mater. Chem. 6, 14420 (2018)
[3] Huang et al., J. Phys. Lett. 12, 2721 (2021)
[4] Bocchini et al., Phys. Rev. Materials 6, 105401 (2022)

HL 36.52 Wed 18:00 Poster E

Atomic Layer Deposition of Pt-doped Ta_2O_5 Coatings for Photoelectrochemical Water Splitting — •Julius Kleusberg[1,2], Tim Rieth[1,2], Guanda Zhou[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]TUM School of Natural Sciences, TU Munich, Garching, Germany

Photoelectrochemical (PEC) water splitting provides a promising avenue for transitioning from a fossil fuel-based economy towards low-carbon alternatives. In PEC devices, photoabsorbers are immersed into an electrolyte, absorb light, generate and separate electron-hole pairs, and thereby drive the water splitting reactions. However, the chemical instability of many efficient photoabsorbers under PEC conditions remains a critical challenge. Consequently, a quest for functional coatings protecting the photoabsorber arise. Tantalum oxide (Ta_2O_5) emerged as promising protective material due to its high electrochemical inertness and full transparency to the solar spectrum. However, as wide bandgap semiconductor, Ta_2O_5 suffers from low electrical conductivity that prevents efficient charge transport to the catalytic surface. In this study, we introduce Pt sub-cycles in a Ta_2O_5 ALD process to achieve Pt-doped Ta_2O_5 thin films with enhanced electrical conductivity. We tailor the Pt-concentration via the sub-cycle ratio and thereby introduce additional states at the valance band edge that shift the Fermi-level downwards. Finally, we apply the developed Pt-doped Ta_2O_5 coatings on $BiVO_4$ photoanodes, analyse PEC improvements, and, ultimately, demonstrate doped ALD coatings as a promising way towards durable photoelectrochemical water splitting.

HL 36.53 Wed 18:00 Poster E

Exploring spin-dependent transport in $BiVO_4$ — •Sven Doll, Melina Pees, David Vogl A., Noah Braitsch, Ian D. Sharp, and Martin S. Brandt — Walter Schottky Institut and School of Natural Sciences, Technische Universität München, 85748 Garching, Germany

Bismuth vanadate $BiVO_4$ is a promising photoanode material for solar-to-fuel conversion. This semiconductor is particularly interesting considering its strong visible light absorption, efficient charge carrier separation, and favorable quasi-Fermi-level alignment with relevant redox potentials. However, small polaron transport strongly reduces its performance. To gain further insight into the charge carrier transport by these polaronic states, we explore whether we can observe a spin dependence of the hopping of the small polarons in $BiVO_4$ using electrically detected magnetic resonance (EDMR). We investigate polycrystalline thin films grown by metal-organic decomposition on conductive and non-conductive transparent substrates. Furthermore, we prepared different electrical contact configurations via physical vapor deposition to analyze in-plane and out-of-plane transport in this material and to achieve small resistances and RC time constants to meet the experimental requirements of EDMR. Since spin-dependent signals are known to critically depend on the charge carrier density (e.g., from similar experiments on doped crystalline silicon), we evaluate the possibility of using the persistent photoconductivity of $BiVO_4$, as well as the introduction of donors in the form of oxygen vacancies and hydrogen impurities, to tune the polaron density.

HL 36.54 Wed 18:00 Poster E

Photoelectrochemical CO_2 reduction with co-catalysts on atomic layer deposited titania protection layers — •Giovanni Postacchini[1,2], Julius Kühne[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Light-driven CO_2 reduction is a promising approach to sustainably address increasing anthropogenic CO_2 emissions and meet the ever-increasing energy demand through the production of solar fuels. However, in an electrochemical environment, the semiconductor photoabsorber must be chemically protected against harsh reaction conditions. Atomic layer deposited (ALD) titania is an optimal candidate for photocathode corrosion protection layers thanks to its chemical stability, passivating effect, and optical transparency in the visible/infrared spectrum. Here, different Ag co-catalyst thin layers are deposited on titania-protected photoabsorbers. The photocathodes are characterized by photoelectrochemical (PEC) measurements using a three-electrode setup in a two-compartment cell to assess the photoelectrocatalytic activity and stability under CO_2 reduction conditions. Gas chromatography (GC) measurements allow the quantification of the product gases and determination of the selectivities of photoanodes towards desired reaction products. Further ex-situ AFM, SEM and XPS analyses are conducted to study surface morphology and composition changes and to elucidate possible degradation mechanisms.

HL 36.55 Wed 18:00 Poster E

Challenges in optical detection of high-amplitude deflections of micro- and nanomechanical systems — •Jannik Dornseiff, Mengqi Fu, Fan Yang, and Elke Scheer — Universität Konstanz, Deutschland

Micro-electro-mechanical systems (MEMS) and their behavior in the nonlinear, high amplitude regime have gathered great interest for research as well as for many engineering applications, like signal processing [1] and amplification [2], mass sensing [3], displacement measurement [4] and more. Optical detection methods, like digital holography microscopy (DHM) or Michelson interferom- etry are versatile and efficient methods of investigating MEMS, but they come with challenges, particularly when it comes to the calibration of the deflection amplitude [5]. By comparison of the results obtained with different instruments, acquisition schemes and analysis methods [6, 7] we are able to identify artifacts, arising from the nonlinear optical transduction when the deflection amplitude overcomes a certain fraction of the optical wavelength used for the detection. We give several examples and also discuss mitigation strategies to minimize these artifacts.

[1] Erbe A et al Appl. Phys. Lett. 77 3102-4 (2000); [2] Almog R et al Appl. Phys. Lett. 88 213509 (2006); [3] Buks E and Yurke B Phys. Rev. E 74 046619 (2006); [4] Trusov A and Shkel A J. Micromech. Microeng. 17 1583-92 (2007); [5] Dolleman RJ et al Appl. Phys. Lett. 111 253104 (2017);[6] Waitz R et al Phys. Rev. B 85 035324 (2012); [7] Yang F et al Sensors and Actuators A: Phys. 354 114307 (2023)

HL 36.56 Wed 18:00 Poster E

Enhancement of wurtzite AlN by ion beam strain engineering: experiments and simulations — •Florian Fuchs[1,2], Holger Fiedler[3], John V. Kennedy[3], and Jörg Schuster[1,2] — [1]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [3]National Isotope Centre, GNS Science, Lower Hutt, New Zealand

We study the piezoelectric properties of wurtzite AlN, and in particular the enhancement of these properties by noble gas [1] and transition metal interstitials.

Using ion-beam implementation, Ne, Ar, Xe, Ti, Zr, and Hf ions were implanted. The measurements show a massive increase in the d_{33} component of the piezoelectric tensor of up to 30% when using Ar^+ or Ti^+. Scanning transmission electron microscopy was utilized to characterize the underlying structure after ion-implantation, demonstrating the occurrence of different interstitial types and the formation of chemically inaccessible noble-gas containing materials.

Density functional theory was used to calculate formation energies of the noble gas interstitials, showing that larger noble gases require a larger formation energy. The most stable positions of the interstitial within the AlN lattice were also determined. Finally, the piezoelectric tensor was calculated and compared to the experimental measurements.

[1] H. Fiedler et al., *Adv. Electron. Mater.* **7**, 2100358 (2021)

HL 36.57 Wed 18:00 Poster E

Theoretical Study on the Cubic (In, Ga)N Random Alloy and Ordered Structures — •Christian Maas[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Through variation in the composition x of indium gallium nitride $In_xGa_{1-x}N$, the band gap can be engineered over the full visible spectrum. By utilizing the cubic zincblende structure, the presence of polarization fields can be avoided intrinsically. Otherwise, these fields could have a negative impact on certain properties, for instance the efficiency of LEDs.

In general, (In,Ga)N is a random alloy, even though there are recent reports on an CuPt-type ordering at certain compositions. We apply the coherent potential approximation (CPA)[1] to describe the random alloy for any given composition. To properly predict the fundamental electronic band gap, we use the low computational cost LDA-1/2 method [2]. In this study, we present our results on structural and electronic properties such as stability, lattice parameter, band gap and phonon modes for the random alloy and certain ordered structures such as the CuPt-type ordering.

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

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

HL 36.58 Wed 18:00 Poster E

Temperature dependent free carrier concentration in GaN:Si — •Christina Harms, Jona Grümbel, Rüdiger Goldhahn, and Martin Feneberg — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany

GaN is already commercialized in a variety of different applications. Nevertheless, still fundamental questions remain to be answered. Here, we focus on the temperature dependence of the free carrier concentration of doped GaN. We investigate the Raman excitations of hexagonal bulk GaN:Si from 80 K to 300 K. Six samples with carrier concentrations ranging from 10^{12} to 10^{19} cm^{-3} were measured using laser excitation at 532 nm. Our results reveal that at room temperature, both coupled phonon-plasmon modes ($LPP_{\pm}$) are visible and agree with Hall-effect experiments. Under temperature variation, the LPP_+ mode shows a weak frequency shift or remains even unaffected. Surprisingly, the LPP_- mode exhibits a frequency shift towards higher frequencies with decreasing temperatures for all samples, contradicting previous assumptions. To shed light onto this shift, photoluminescence spectra are taken into account as well. The combination of both experimental data sets allows to better understand the evolution of temperature dependence of the free carrier concentration.

HL 36.59 Wed 18:00 Poster E

Electrical characterization of n-GaN nanowires to n-Si(111) growth substrates with AlN interlayer — •Juliane Koch[1], Patrick Häuser[2], Peter Kleinschmidt[1], Werner Prost[2], Nils Weimann[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]University of Duisburg-Essen, Components for High Frequency Electronics (BHE), Duisburg, Germany

III-V semiconductor nanowires (NW) have demonstrated high potential as building blocks in a wide range of applications in electronic and optoelectronic devices. In particular, GaN-based nanowires have attracted attention in recent years, especially in the field of UV-LEDs and sensors. For the realization of these devices, special attention must be paid to the surfaces and interfaces, since the electrical properties can be strongly influenced by the surface properties and the sequence of layer deposition. A detailed electrical investigation is therefore necessary, which was done by a four-point measurement method using a multi-tip scanning tunnelling microscopy (MT-STM). For this purpose, we investigate in this work single GaN NWs in an upright standing configuration applying a MT-STM and a built-in scanning electron microscope. We focus on the limiting factors of the current in GaN NWs on an n-doped Si(111) substrate. Our detailed investigations reveal the NWs themselves are highly conductive and that the NW-to-substrate junction as the limiting factor, dominating the overall electrical behavior. The impact of the junction is strongly dependent on the thickness and crystal structure of the AlN layer.

HL 36.60 Wed 18:00 Poster E

Atomic structure of As-modified Si(100) surfaces prepared in MOCVD ambience utilizing background arsenic — Chris Yannick Bohlemann[1], Agnieszka Paszuk[1], Manali Nandy[1], Aaron Flötotto[2,3], Max Grossmann[2,3], Oleksandr Romanyuk[4], •Kai Daniel Hanke[1], Peter Kleinschmidt[1], Erich Runge[2,3], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials — [2]TU Ilmenau, Institute of Physics,Theoretical Physics I — [3]TU Ilmenau, Centre of Micro- and Nanotechnologies — [4]Institute of Physics, Academy of Sciences of the Czech Republic, 182 00 Prague 8

A low-defect III-V nucleation layer and a well-defined atomically abrupt interface between the Si(100) substrate and the III-V nucleation layer are essential prerequisites for subsequent low-defect III-V layer growth. Preparation of a well-ordered Si(100) surface in industrially-relevant MOCVD ambience with arsenic benefits in a significant temperature reduction during the deoxidation step. In this study, we investigate the atomic structure of Si(100) surfaces prepared in As-rich MOCVD reactor, employing background arsenic as the arsenic source. The preparation of the samples in the MOCVD reactor was monitored in situ by surface sensitive optical spectroscopy and the surfaces were characterized in UHV by FTIR and STM. The measurements are supported by complementary DFT calculations. We confirm presence of hydrogen on the surface and mixed As-Si-H dimers, which was previously unrecognized.