TT 66: 2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

TT 66.1 Wed 18:00 P2

Observation of many-body-localization in substituted 1*T*-TaS_2 — •Jesumony Jayabalan[1], Gael Reecht[1], Ricards Kristers Knipšis[2], Florian K Diekmann[3], Friedemann Queisser[2], Walter Schnelle[4], Ping Zhou[1], Kai Rossnagel[3], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Uni. of Duisburg-Essen, Fakultät für Physik and CENIDE — [2]HZ Dresden-Rossendorf, — [3]CAU of Kiel and DESY — [4]MPI for Chemical Physics of Solids, Dresden

Random modulations in the potential landscape are known to localize a single quantum particle, the Anderson localization leads, to stable non-thermalizing states. Adding interaction is expected to cause delocalization and a quick thermalization of such single particles, but in a strongly disordered system, the many-body quantum state itself becomes localized, known as the Many-Body Localization (MBL). Using time-resolved photoelectron spectroscopic measurements, we show that it is possible to realize MBL states in a Tungsten substituted 1*T*-TaS_2 material. Electrons are excited by using a 1.51 eV, 50 fs pulses and a 6 eV probe pulse was used to photoemit electrons. In contrast to ultrafast (<20 fs) decay of doublons in pristine 1*T*-TaS_2[1], we observe that some of the doublons decay in hundreds of femtosecond time scale, while the rest lasts for more than few microseconds. This observation is supported by scanning tunneling microscopic measurements and Fermi-Hubbard model calculations. Funding by DFG through QUAST-FOR5249 and SFB 1242 is acknowledged. [1] M. Ligges et al., Phys. Rev. Lett., 120, 166401 (2018).

TT 66.2 Wed 18:00 P2

Exciton Transport in Monolayer TMDs — •Lifeng Ou, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV, University of Valencia, Valencia, Spain

Atomically thin transition metal dichalcogenides semiconductor emerges as promising candidates for novel optoelectronic application, displaying weak dielectric screening due to its truly two-dimension character. The optical properties are mostly related to inter-band transitions between valence and conduction bands, also called the strongly binding electron hole pair, exciton. Strain is expected to impact spatiotemporal distribution of excitons, e.g. spatially inhomogeneous strain acts as a driving force for exciton/carrier funneling, similarly to bias fields for charged particles. In this work we demonstrate the capability to manipulate exciton motion via spatially modulated strain fields, where excitonic energy especially its bandgap is largely tunable and the effective mass of electronic valleys is modified resulting in a qualitative change of the excitonic landscape and efficiency of exciton-phonon scattering channels. These transport properties are represented by the coupled two equations, continuity equation and drift-diffusion equation, which derive from zero-order and first-order moment of Boltzmann equation, respectively. In addition, the simulation diffusion coefficient and mobility in latter equation are evaluated by first-principle and experiment qualitatively, as the function of strain fields.

TT 66.3 Wed 18:00 P2

trARPES investigation electron-phonon coupling in CrSBr — •Maurits Houmes, Karl Schiller, Lasse Sternemann, Jonah Nitschke, and Mirko Cinchetti — Departement of Physics, TU Dortmund University, 44227 Dortmund, Germany

CrSBr is a magnetic, semiconducting van der Waals material that has recently attracted significant interest. It hosts both localized Frenkel excitons and delocalized Wannier-Mott-like excitons, and its excitonic properties are strongly influenced by magnetic ordering and lattice distortions. [1,2,3] These features make CrSBr a compelling platform for exploring correlated phenomena in condensed matter systems.

To advance our understanding of the interplay between excitons, magnetism, and lattice dynamics in this material, a more complete characterization is essential. In this work, we present time- and angle-resolved photoemission spectroscopy (trARPES) measurements performed on CrSBr, with particular emphasis on quantifying the electron-phonon coupling. Aiming to provide a previously missing component needed to build a comprehensive picture of the interactions in CrSBr, offering a foundation for future studies and potential technological applications of this promising material.

1. Smiertka, M. et al. Preprint at ArXiv:2506.16426 (2025). 2. Lin, K. et al. ACS Nano 18, 2898-2905 (2024). 3. Bork, S. et al. Preprint at ArXiv:2511.20268v1 (2025).

TT 66.4 Wed 18:00 P2

Probing defect-induced wave patterns and superconductivity in 2*H*-NbS_2 — Werner M.J. van Weerdenburg, •Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) host a variety of electronic phases, including superconductivity and charge-density-wave (CDW) order. Recent reports on 2*H*-NbS_2 have added a coexisting pair-density-wave (PDW) order to this set, inspiring new questions about the coexistence and driving mechanisms of these phases [1]. In contrast, the closely-related superconducting compound 2*H*-NbS_2 lacks a CDW phase, but has been suggested to be close to a CDW instability and sensitive to the presence of defects [2,3].

Using low-temperature scanning tunneling microscopy and spectroscopy, we probe the electronic, phononic and superconducting properties of 2*H*-NbS_2. We observe wave-like modulations around intrinsic defects in differential-conductance maps and compare them to band-structure calculations. To assess the nature of these modulations, we probe the modulated regions and characterize the superconductivity spatially. These observations add to the ongoing exploration of superconducting, CDW, and PDW phases in TMDC materials.

[1] Liu et al., Science 372,1447-1452 (2021); [2] Heil et al., PRL 119, 087003 (2017); [3] Wen et al., PRB 101:241404, 6 (2020)

TT 66.5 Wed 18:00 P2

Theory of few- and many-body excitations in carbon nanotubes — •Maurice Beringuier[1,2] and Richard Schmidt[1,2] — [1]Institut für Theoretische Physik, Philosophenweg 16, 69120 Heidelberg — [2]Universität Heidelberg, Grabengasse 1, 69117 Heidelberg

Even decades after their discovery, some properties of Carbon Nanotubes (CNTs) are still not fully understood. One of the phenomena still lacking a satisfying explanation is the behaviour of the absorption spectrum of semiconducting CNTs under doping. A resonance in these spectra appears only in the presence of additional charge carriers.

This has in the past been described with phenomenological models or few body physics (using trions and excitons), but experimental data (e.g. time resolved measurements of the spectra) hint at potential signatures of many-body physics. Inspired by their abundance in 2D or 3D semiconductors and cold quantum gases, we investigate whether quasiparticles like Fermi polarons could be responsible for the observations in CNTs, which due to their interesting geometry exhibit aspects of both 1D and 2D materials.

We tackle these questions by modeling charge carriers and excitons on CNTs interacting using a combination of exact diagonalization and variational techniques to gain insight into the interplay of few- and many-body physics in these systems.

TT 66.6 Wed 18:00 P2

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

In recent years, the rising class of non-van der Waals 2D materials [1] has garnered substantial attention for their distinctive electronic and magnetic properties. In this contribution, we explore the impact of spin-orbit coupling (SOC) on the properties of these non-van der Waals 2D systems and its potential to induce topological properties. Given the presence of heavy elements like Bi and Tl in several 2D candidates, SOC effects notably influence the electronic structure. In our approach, we utilize AFLOW's standardized workflows [2] for initial screening. Subsequently, we extract metadata using AFLOW and tailor the parameters with an AiiDA-plugin [3] for precise electronic structure calculations employing the full-potential all-electron program FLEUR [4] within AiiDA. We analyze the influence of SOC on band structures and densities of states, with a particular focus on topologically protected 1D conduction edge channels.

[1] R. Friedrich *et. al.*, Nano Lett. **22**, 989 (2022).
[2] Divilov *et. al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.

TT 66.7 Wed 18:00 P2

Strain Engineering Single Photon Emission in hBN and MoS2 Monolayers using First Principles — •Paulina Chodyra, Chengcheng Xiao, Johannes Lischner, and Arash Mostofi — Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K

Point defects in monolayer hexagonal boron nitride (hBN) and molybdenum disulphide (MoS_2) are promising single-photon emitters (SPEs) for quantum technologies due to their potential for room-temperature operation and high photon emission efficiency. In this work we use density-functional theory calculations to investigate the nitrogen antisite-vacancy complex (N_BV_N) and boron vacancy (V_B) in hBN, and the sulphur vacancy (V_S) in MoS_2. We calculate the defect formation energy of different charge states of these defects as a function of biaxial strain and electronic chemical potential. For the charge states that are likely candidates for SPE, we find that their stability can be enhanced via application of biaxial strain. Furthermore, the range of electronic chemical potential over which these charge states are stable can also be increased. These findings can provide predictive design rules for strain-engineered SPEs with improved resilience against electrostatic fluctuations. It also establishes our first steps toward an accelerated discovery of stable SPEs across 2D materials, where DFT-derived stability criteria combined with optical absorption and emission spectra could enable a deeper understanding of SPE operation under realistic conditions.

TT 66.8 Wed 18:00 P2

Beyond the Gamma point: Scanning tunneling spectroscopy on MoS_2/graphene/Ir(111) — Borna Pielić[1,2], Dino Novko[2], Nina Girotto Erhardt[2], Vito Despoja[2], Alice Bremerich[1], Sumanasa Begur Prakash[1], •Robin Ohmann[1], and Carsten Busse[1] — [1]Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany — [2]Institute of Physics, Bijenička cesta 46, 10000 Zagreb, Croatia

Scanning tunneling spectroscopy (STS) reveals information about the band structure of surfaces by measuring the local density of states, and it also allows detection of quasiparticles. For semiconducting transition-metal dichalcogenides the conduction- and valence-band edges have been readily explored with this method. However, STS studies at higher energies than the Γ-point are limited. Here, we investigate epitaxially grown monolayer islands of MoS_2 on graphene/Ir(111) using STS at low-temperature (T=10 K). Specifically, we employ the constant-current STS method, which enables easier access to spectroscopic features with higher energies, than the more commonly used constant-height STS. We find several peaks a few hundred meV above the Γ-point. We do not see them on graphene, allowing us to exclude substrate- or tip-related effects. When measured near the step edge of an island, these peaks bend closer to the Fermi level, similar to the peak at the Γ-point. Their appearance also varies depending on tip condition and intercalation. Our observations cannot be explained in a single-particle picture. Possible many-body models, such as phonon assisted inelastic tunneling or plasmarons are discussed.

TT 66.9 Wed 18:00 P2

Band structure and Work Function in Ultrathin HfSe2 — •Young Jun Chang — University of Seoul, Seoul, Republic of Korea

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit significant modifications in their electronic structures when reduced from bulk to monolayer thickness. In this study, we investigated the thickness-dependent electronic properties of epitaxial 1T-HfSe2 thin films. The films were grown via molecular beam epitaxy (MBE) and monitored in situ by reflection high-energy electron diffraction (RHEED). Scanning tunneling microscopy (STM) revealed atomically flat surfaces with well-defined 1T hexagonal lattices, while scanning tunneling spectroscopy (STS) measured a bandgap of ˜1.1 eV for the monolayer. Angle-resolved photoemission spectroscopy (ARPES) revealed thickness-induced band splitting in the valence band, while the valence band maximum (VBM) remained pinned regardless of thickness. In contrast, the work function increased monotonically with film thickness. Density functional theory (DFT) calculations reproduced the observed band structures and attributed the thickness-dependent work function to the screening effect of the underlying graphene substrate. These findings provide key insights into band alignment and interface engineering in 2D semiconductor-based electronic and optoelectronic devices. (RS-2023-00220471, RS-2023-00284081, RS-2024-00334854)

TT 66.10 Wed 18:00 P2

Exciton and trion dynamics of 2D transition metal dichalcogenides — •Seawoo Moon[1], Alessandro De Vita[1], Lawson T. Lloyd[2], Tania Mukherjee[1], Anh T. Nguyen[3], Dong-Wook Kim[3], Martin Wolf[2], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1] — [1]Institute for Physics and Astronomy, TU Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Germany — [3]Department of Physics, Ewha Womans University, South Korea

Key functionalities of transition metal dichalcogenides (TMDs) are determined by excitons whose behaviour can be tweaked by interface–induced external perturbation such as proximity effects, charge transfer and local electromagnetic fields. Excitonic behaviors and band alignment of TMDs with interfacing materials are explored. We studied the band alignment of monolayer WS_2 on nanostructured Ag by Kelvin probe force microscope, a tool that can map electrical potential of sample surface. By this method, the exciton–to–trion conversion mechanisms in WS_2 could be explained, including the role of the localized surface plasmons. For a more direct approach, time and angle–resolved photoemission spectroscopy (TrARPES) with pump–probe technique is employed to directly map the equilibrium and non–equilibrium electronic structure of TMD–metal and TMD/TMD interfaces. In–situ and ex–situ techniques are required to achieve pristine TMD surfaces and interfaces, since TrARPES is a highly surface sensitive technique.

TT 66.11 Wed 18:00 P2

Ultrafast Photocarrier-Induced Ionic Rearrangement in Monolayer ReS_2 Probed with Femtosecond Electron Diffraction — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Martin Wolf[1], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Rhenium disulphide (ReS_2) exhibits a distorted crystal structure compared to prototypical hexagonal transition metal dichalcogenides. This Peierls-like distortion results in quasi-1D chains of Re ions running in plane through each layer of ReS_2, which give rise to prominent anisotropic properties, such as polarization dependent optical absorption and anisotropic effective carrier masses.

We investigate the ultrafast lattice dynamics of monolayer ReS_2 with femtosecond electron diffraction (FED). Leveraging the strength of FED as a direct and quantitative measurement of the crystal lattice, we fit the intensities of many hundreds of Bragg peaks at each time delay to extract time resolved crystallographic information.

With this method, we not only resolve the increase in the incoherent phonon population (Debye-Waller), but also reveal a concerted atomic rearrangement within the lattice, with the ions rapidly (< 1 ps) moving away from their equilibrium atomic coordinates and returning on timescales of a few picoseconds. We associate this response with the aforementioned distortion, and discuss the physical origin.

TT 66.12 Wed 18:00 P2

Exploring Zincblende (100) Semiconductor Surfaces as Platforms for Correlated Adatom Lattices — •Olga Kashirina, Niklas Enderlein, and Philipp Hansmann — Friedrich-Alexander-Universität Erlangen-Nürnberg

Adatom lattices on (111) surfaces of zincblende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting strong electronic correlations and associated emergent behavior near the Fermi energy (see [1] and references therein). Our recent study [2] reveals transition metals adatom lattices on 3C-SiC(111) surfaces to be intriguing candidates for strongly correlated material design. In the present contribution we continue this strategy by leaving the hexagonal/triangular lattices. Specifically, we explore the (100) surfaces of silicon, diamond, and 3C-SiC which in the infinite bulk exhibit a fourfold rotoinversion symmetry enabling square/rectangular adatom lattices. As the (100) surface is prone to dimerization, an additional complication arises from dimer-derived electronic states inside the bulk gap, which - depending on the chosen adatom and substrate combination - may or may not hybridize with the adatom states. In this context, the adatom coverage is another crucial parameter as it directly influences the nature of surface reconstructions and dimer-

izations. To assess the structural stability of our candidate systems, we employ phonon calculations based on density-functional perturbation theory as well as molecular-dynamics simulations. [1] X. Cao, et al., PRB 97, 155145 (2018). [2] H. Menke, N. Enderlein, et al., arXiv:2410.17165.

TT 66.13 Wed 18:00 P2

Engineering correlated electrons in adatom lattices on semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project, we explore promising adatom lattices on semiconducting/insulating substrates such as SiC and cubic BN in order to realize one-, two-, and three-band Hubbard models at different fillings. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field. [1] H.Menke, N.Enderlein, *et al.*, arXiv:2410.17165.

TT 66.14 Wed 18:00 P2

Investigation of the atomic and electronic structures of WSe2-xTex — •Ganbat Duvjir[1], Nguyen-Hoang Dang[2], Younghun Hwang[1], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Electricity and Electronics and Semiconductor Applications, Ulsan College, Ulsan 44610, Republic of Korea

Ternary transition metal dichalcogenides (TMDs) exhibit diverse crystal structures and electronic properties depending on their composition. In this study, we systematically investigate the atomic and electronic structure of ternary WSe2-xTex as a function of Te concentration using scanning tunneling microscopy/spectroscopy (STM/S). Notably, STM topography indicates that increasing the Te content induces structural deformation of the hexagonal lattice of WSe2-xTex. This deformation manifests as the stretching of 2H structure along the zigzag direction and compression along the armchair direction. STS measurements reveal a significant reduction in the band gap of WSe2-xTex with increasing Te concentration. While the valence band maximum shifts toward the Fermi level, the conduction band minimum remains relatively unchanged.

TT 66.15 Wed 18:00 P2

STM study on tuning the Fermi level of transition metal dichalcogenides — •Nguyen-Hoang Dang[1], Mincheol Kim[2], Ganbat Duvjir[1], Young Jun Chang[2,3], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Department of Physics, University of Seoul, Seoul 02504, Republic of Korea — [3]Department of Smart Cities, University of Seoul, Seoul 02504, Republic of Korea

Controlling the Fermi level is essential for tailoring the electronic properties of semiconductors. Here, we investigate two routes of chemical doping and defect control using scanning tunneling microscopy and spectroscopy. For V-doped $MoSe_2$, we study how substitutional V atoms influence its electronic structure. Although STM primarily probes the top Se layer and the dopants are not directly imaged, the topography exhibits defect-like features whose contrast reverses with the bias polarity: dark at positive sample bias and bright at negative bias. This is characteristic of negatively charged acceptor states, consistent with V substituting Mo. STS spectra show a Fermi-level shift toward the valence band, indicating that V doping drives $MoSe_2$ from intrinsic n-type toward p-type. For $HfSe_2$, we study defect control via thermal annealing. STS measurements under different annealing conditions show Fermi level shifts toward the conduction band, suggesting that prolonged annealing enhances Se-vacancy formation, which acts as an electron donor. These results highlight how STM/STS links local defects with electronic properties, offering microscopic insight into Fermi level tuning through doping and defect engineering.

TT 66.16 Wed 18:00 P2

Impact of Mo doping on the charge density wave in 1T-TaS_2 studied by laser-ARPES and LEED — •Adina Timm[1,2], Finja Schillmöller[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Controlling charge density waves (CDWs) in quantum materials enables the fine-tuning of their electronic properties, paving the way for future electronic and optoelectronic devices. The layered compound 1T-TaS_2 exhibits various temperature-dependent CDW phases that we aim to modify through doping. We introduced the dopant molybdenum during crystal growth via the chemical vapor transport method. Using 11-eV laser-based angle-resolved photoelectron spectroscopy (ARPES), we comparatively measured the electronic band structures of pristine and Mo-doped 1T-TaS_2 crystals. Complementary low-energy electron diffraction (LEED) measurements revealed the structural rearrangements during the CDW transitions and partial CDW suppression at specific doping levels. Our results suggest that modest Mo doping allows for subtle adjustments to the CDW landscape of 1T-TaS_2, yielding different transition temperatures while preserving the underlying electronic-structural order.

TT 66.17 Wed 18:00 P2

Probing Electronic Structure Modulation in WSe_2 and $MoTe_2$ under Out-of-Plane Electric Fields via ARPES and XPS — •Sonja Reinheimer[1,2], Lukas Bruckmeier[1,2], Jakob Dilling[1,2], Jens Buck[1,2], Matthias Kalläne[1,2,3], Chithra Sharma[1,2,4], Markus Scholz[5], and Kai Rossnagel[1,2,3] — [1]IEAP, CAU Kiel, 24098 Kiel, Germany — [2]RHL, DESY, 22607 Hamburg, Germany — [3]KiNSIS, CAU Kiel, 24098 Kiel, Germany — [4]Universität Hamburg, 22761 Hamburg, Germany — [5]DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are quantum materials that exhibit a broad spectrum of emergent electronic phenomena, arising from layer-dependent band structures. Owing to their tunable (opto-)electronic properties, TMDCs are promising candidates for next-generation photovoltaic devices and highly integrated electronic components. A key challenge is to systematically control charge transport and band alignment in these layered systems. Here, we investigate vertically stacked 2H-WSe_2/2H-$MoTe_2$ heterostructures using angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy. By performing in-operando ARPES on a sample with an applied out-of-plane electric field during the measurements, we can directly probe field-induced modifications to the electronic band structure and the density of states. This approach enables us to identify electric-field-driven changes in the electronic and lattice structure and contribute to a deeper understanding of electric control mechanisms in TMDC heterostructures.

TT 66.18 Wed 18:00 P2

Many-body localisation in the Fermi-Hubbard model? — •Ričards Kristers Knipšis[1], Jesumony Jayabalan[2], Gael Reecht[2], Vivek Mondal[2], Florian Konstantin Diekmann[3], Friedemann Queisser[1], Ping Zhou[2], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[1,6], Manuel Gruber[2], and Uwe Bovensiepen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-University of Kiel, Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]Ruprecht-Haensel-Laboratory, DESY, Hamburg, Germany — [6]Institute of Theoretical Physics, Dresden University of Technology, Dresden, Germany

Motivated by recent experimental results, we study the 2D Fermi-Hubbard model in the Mott insulator state under the influence of a disorder potential. Special emphasis is placed on signatures of many-body localisation.

Using the hierarchy of correlations, we find that the disorder potential can localise the effective quasi-particle wavefunctions, resulting in their spatial separation. This, in turn, can be used to explain the drastic increase in the quasi-particle lifetimes observed in experiment.

Funding by the DFG through the SFB 1242 is gratefully acknowledged.

TT 66.19 Wed 18:00 P2

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Robert Zierold[4], Tim Riedel[1,2], Adina Timm[1,2], Robert H. Blick[4], and Kai Rossnagel[1,2,3] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]RHL, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]CHyN, Universität Hamburg, 22761 Hamburg, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a quasi-two-dimensional hexagonal $2H$ structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping. This makes it a highly attractive candidate for spintronic applications. Density functional theory calculations and scanning transmission electron microscopy studies support this assumption, and RKKY interactions are predicted to be the driving mechanism. Pristine WSe_2 and vanadium-doped WSe_2 crystals were synthesized in separate in-house batches using the chemical vapor transport (CVT) method. The doped samples were grown with varying nominal concentrations of V intended to induce substitutional doping at the tungsten sites. The samples were investigated using a vibrating-sample magnetometer (VSM). The results provide insight into the magnetic characteristics of the doped material compared to the pristine reference crystal.

TT 66.20 Wed 18:00 P2

Coexistence of a fully metallic antiphase boundary and the semiconducting charge density wave phase in 1T-TaS_2 — •Georg A. Traeger[1], Kai Rossnagel[2,3], and Martin Wenderoth[1] — [1]IV. Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Transition metal dichalcogenides are an ideal platform for studying the interplay between charge density waves (CDWs), electronic correlations, and defect states. Using scanning tunneling microscopy and spectroscopy, we investigate a new type of intrinsic antiphase boundary (APB) in the commensurate CDW phase of 1T-TaS_2. In contrast to previous studies, we find a metallic APB extending laterally across several nanometers. We observe evanescent states spilling out from the defect into the metallic region and find that the fingerprint of the semiconducting system gradually disappears within the APB, without signs of strong interactions, suggesting the orthogonality of the two systems wave functions. Our findings highlight the crucial role of domain boundaries in the interpretation of other, especially conductivity-based, measurements. Furthermore, we propose this new type of metallic APB as a model system to study interlayer coupling in correlated layered materials.

TT 66.21 Wed 18:00 P2

Temperature-dependent VUV-ARPES of 1T-$Mo_xTa_{1-x}S_2$ — •Torben Petersen[1,2], Matthias Kalläne[1,2,3], Adina Timm[1,2], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Examining the charge density wave (CDW) phase transitions of transition metal-substituted transition metal dichalcogenides (TMDCs) provides insight into tuning transition behavior by doping. To this end, we use the 1T-$Mo_xTa_{1-x}S_2$ reference system, comparing the pristine sample with two doped samples (x = 0.5% and x = 1%) using 11 eV laser-based VUV-ARPES. We investigate work function changes alongside doping-induced band structure changes in the temperature range of 60 K to 370 K. This allows us to observe the high- and low-temperature CDW phase transitions known from the pristine material and determine how the CDW-induced band structure changes vary with doping.

TT 66.22 Wed 18:00 P2

STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111) — •Alina Drechsler, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDs) exhibit thickness-dependent electronic properties and are highly sensitive to structural defects, which can strongly modify their density of states even at low concentrations. Defect engineering has therefore become an important route to tailor their electronic, magnetic, optical, and catalytic behaviour. While most of the current research focuses on naturally occurring defects in chemical vapour-deposited TMDs, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE) to improve control in defect engineering.

We present scanning tunneling microscopy and spectroscopy (STM/STS) studies of Fe-doped monolayer MoS_2 on Gr/Ir(111), achieved by co-evaporation Fe during MBE growth. By comparing to undoped MoS_2 grown under identical UHV conditions, we identify the Fe-related defects and measure their electronic signatures. STS reveals in-gap states associated with single-atom Fe inclusions, whose spatial distributions are resolved via differential conductance mapping. Additionally, resonant tunneling spectroscopy shows that Fe inclusions modify the image potential states by locally shifting their energetic positions. Our work demonstrates the potential of single-atom substitutions for tailoring the electronic properties of two-dimensional TMDs.

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Layer thickness dependent band gap of MBE grown single- to few-layer MoS_2 — •Maciej Bazarnik[1], Marta Przychodnia[1,2], Thorsten Deilmann[3], and Anika Schlenhoff[1] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Physics, Poznan University of Technology, Poland — [3]Institute of Solid State Theory, University of Münster, Germany

In light of the rise of transition metal dichalcogenides as 2D semiconductors for device applications, band engineering becomes very important from an application point of view. In many of these materials, such as the canonical example of MoS_2, the semiconductor band gap depends on the layer number. There is a transition from an indirect band gap semiconductor in bulk to a direct band gap for a monolayer. Interestingly, it was predicted and experimentally confirmed that, by thinning the material from bulk to a bilayer, the indirect transition blue-shifts.

Here, we present the results of scanning tunnelling spectroscopy measurements on MoS_2 that has been grown in situ via molecular beam epitaxy (MBE) on graphene on Ir(111) at thicknesses ranging from 1 to 6 layers. We observe a decrease in the band gap with increasing layer number. We also find a pinning of the conduction band, which vanishes for layer thicknesses beyond 4 layers. Comparing our experimental data with DFT and GW calculations indicates that a screening in addition to that of the substrate needs to be introduced to explain the experimentally obtained relation. We discuss possible sources of this additional screening in light of our findings.