TT 65: 2D materials: Stacking and heterostructures – Poster (joint session O/TT)

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

TT 65.1 Wed 18:00 P2

Unexpected Ordered Interfaces in WSe_2-$MoSe_2$ Lateral Interfaces Observed by STEM — •Matvei Kislitsyn[1], Max Bergmann[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

Two-dimensional WSe_2-$MoSe_2$ lateral heterostructures offer a platform for engineering band alignment and excitonic behavior through atomic-scale control of composition, making this material attractive for use in 2D optoelectronic devices. In this contribution, we present a systematic scanning transmission electron microscopy (STEM) study of monolayer WSe_2-$MoSe_2$ heterostructures synthesized by chemical vapor deposition (CVD) directly on SiO_2 TEM grids. While some investigated 2D flakes show atomically sharp interfaces with minimal intermixing, we also observe a highly ordered and unexpected interface configuration consisting of alternating Mo and W atomic rows. By comparing experimental observations with STEM image simulations and theoretical predictions, we analyze the structural origins of both interface types and discuss the mechanisms that may give rise to this unusual ordering. These results provide insight into interface formation mechanisms in lateral transition-metal dichalcogenide heterostructures and their potential impact on material properties.

TT 65.2 Wed 18:00 P2

Superdomains and Strain Localization in Twisted Two Dimensional Transition Metal Dichalcogenides — •Riya Patel[1], Daniel Wolf[1], Kristina Weinel[1,2], Silke Hampel[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, 01069 Dresden — [2]Faculty of Physics, Technical University Dresden, 01069 Dresden

Bilayers of 2D transition metal dichalcogenides (TMDCs) exhibit special structural and electronic phenomena when stacked with a low-twist-angle. Particularly, they undergo lattice reconstruction, forming large triangular stacking domains, separated by domain walls that concentrate strain (soliton regime), which was shown in simulations. However, direct experimental quantification of these strain features and their correlation with electronic properties remains limited. Here we investigate low-twist-angle TMDCs using high-resolution transmission electron microscopy to visualize the reconstructed super lattice and identify the resulting superdomains structure. We employ geometric phase analysis to quantitatively map the strain distribution at the domain walls with nanometer resolution, revealing spatial maps of different strain components. We use Electron Energy Loss Spectroscopy to further probe the electronic properties of the reconstructed system. The understanding of strain localization in superdomain structures and the related electronic properties in such systems facilitate strain-engineered electronic properties in twisted TMDCs.

TT 65.3 Wed 18:00 P2

Pseudomonolayer TMDCs via organic intercalation — •Katharina Steinkirchner[1,2], Jakob Dilling[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Markus Scholz[4], and Kai Rossnagel[1,2,3,4] — [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 — [4]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are a versatile class of layered materials with tuneable electronic properties. One approach to tailoring these properties is to manipulate the material's effective dimensionality. Specifically, intercalating cationic organic molecules with different alkane carbon chain into the van der Waals gaps between the layers increases the interlayer distance of the TMDC host material. This transforms the crystal from a bulk state to a monolayer-like state, thereby altering the electronic structure [1]. Here, we present a comprehensive study of the geometric and electronic structures of intercalated and non-intercalated TMDCs, such as $NbSe_2$, using SEM, EDS, and 11eV laser-based ARPES.

[1] H. Zhang *et al.*, Nat. Phys. **18**, 1425 (2022).

TT 65.4 Wed 18:00 P2

Preparation of quasi-freestanding few-layer samples of 2D materials — •Seyedeh Helya Alaei, Hanna Shirin Pulikkal Hamza, Mashood Tariq Mir, Lukas Nöding, Ahmed Hassanien, Arne Senftleben, Jochen Mikosch, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

Two-dimensional (2D) materials have garnered significant attention in the last two decades and have been analyzed using various methods in the fields of materials science and physics. To study the dynamic behavior of 2D materials upon irradiation with femtosecond laser pulses using ultrafast electron diffraction, it is necessary to isolate few-layer structures from bulk crystals and prepare them in a quasi-freestanding manner. Due to the weak van-der-Waals forces between the layers relative to the in-plane forces of the structure, mechanical exfoliation is a commonly used method. However, the transfer is challenging, due to the thinness of the flake and the adhesive force between the flake and the surface. Our preparation involves three major steps: (1) exfoliation using adhesive tape and viscoelastic gel, (2) isolation of 2D material nanosheets with thicknesses ranging from 3 to 50 nm, and (3) transfer onto a standard sample mesh of transmission electron microscopy with a high success rate. The transfer exploits liquid-solid phase transitions of a soluble wax-like material. In this ongoing study, the 2D ferromagnetic material Fe_5GeTe_2 has been of interest. We will discuss the different steps in detail and the challenges associated with the preparation of this material, including the fragility of the crystals due to oxidation and the partially covalent out-of-plane forces.

TT 65.5 Wed 18:00 P2

Ordering Phenomena in MoS_2 Nanocrystals on Graphite — •Lukas Nöding[1], Ahmed Hassanien[1], Mashood Tariq Mir[1], Hanna Shirin Pulikkal Hamza[1], Seyedeh Helya Alaei[1], Thomas Baumert[1], Jochen Mikosch[1], Florian Grassme[2], Claudia Backes[2], and Arne Senftleben[1] — [1]University of Kassel, Institute of Physics, Kassel, Germany — [2]University of Kassel, Institute of Chemistry, Kassel, Germany

Two-dimensional transition-metal dichalcogenides (TMDCs) such as MoS_2 offer a platform for tailoring electronic and optical properties through controlled stacking and orientation. Achieving ordered assemblies of MoS_2 nanocrystals on crystalline substrates is, therefore, of considerable interest. In this work, we study the crystallographic alignment of MoS_2 nanocrystals on a graphite substrate. The samples were prepared using the Langmuir-Schäfer technique, enabling the reproducible deposition of nanocrystals with controlled density. To probe the crystallographic alignment of the deposited nanocrystals with respect to the graphite lattice, we performed wide field static electron diffraction measurements at an acceleration voltage of 35 kV, complemented by selected area electron diffraction at 200 kV.

Our preliminary analysis reveals a pronounced localized and short-range ordered crystallographic alignment of the MoS_2 nanocrystals, extending over at least a few micrometers. A quantitative evaluation of the global ordering behavior, as well as its dependence on crystal size and deposition parameters, is currently underway and will be discussed.

TT 65.6 Wed 18:00 P2

Multiferroic Two-Dimensional Cu(CrX2)2 (X = S, Se, and Te) as Anode Materials for Lithium-Ion Batteries: A First-Principles Study — •Muhammad Fayaz[1] and Zijing Lin[2] — [1]Department of Physics, University of Science and Technology of China, Hefei 230026, China — [2]Department of Physics, University of Science and Technology of China, Hefei 230026, China

Identifying two-dimensional (2D) materials with the desired electrochemical performance for lithium-ion batteries is of great interest in developing next-generation energy devices. Motivated by the successful synthesis of multiferroic 2D materials, Cu(CrX2)2 (X = S, Se, and Te), which exhibit simultaneous ferroelectricity and ferromagnetism, we performed first-principles calculations to investigate their potential as anodes for lithium-ion batteries. We comprehensively investigate the electrochemical properties of the predicted systems and demon-

strate that lithium exhibits sufficient mobility on their surface, with appreciable stability. For instance, the binding energy (Eb) of the lithium adatom on Cu(CrS2)2 is -4.034 eV, with a diffusion barrier as low as 0.212 eV. As a consequence, the maximum theoretical specific capacity for lithium adatoms reaches as high as 1089 and 666 mAhg-1, respectively, for Cu(CrS2)2 and Cu(CrSe2)2, which can be attributed to a much higher storage capacity of lithium adatoms compared to previously identified 2D anode materials. All of these remarkable properties, including high binding energy (Eb), low diffusion barrier, high specific capacity, and good electrical conductivity.

TT 65.7 Wed 18:00 P2

Valence-Band Renormalization and Spin Splitting in a Monolayer WTe2/WSe2 Heterostructure — •Daiyu Geng, Natalie Lehmann, Jiabao Yang, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

Monolayer WTe2 (1L-WTe2) hosts a variety of broken-symmetry phases, including a quantum spin Hall insulator, a topological excitonic insulator, and several intriguing spin-ordered states. The dielectric environment and charge-carrier density play crucial roles in the competition among these electronic phases. In this work, we investigate the band structure of 1L-WTe2 interfaced with semiconducting WSe2 using laser- and synchrotron-based micro-ARPES. We observe strong valence-band renormalization accompanied by pronounced spin splitting in 1L-WTe2. Additionally, multiple replica pockets emerging in the Fermi surface indicate a substantial moiré effect in this heterostructure.