HL 50: 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Thursday 15:00–17:45 Location: H6

HL 50.1 Thu 15:00 H6

Systematic Study of Interlayer Interactions in Transition Metal Dichalcogenide Bilayers Using microARPES — •Thomas Nielsen[1], Chakradhar Sahoo[1], Alfred Jones[1], Zhihao Jiang[1], Kenji Watanabe[2], Takashi Taniguchi[2], Suman Chakraborty[4], Prasana Sahoo[4], Jill A. Miwa[1], Yong P. Chen[1,3], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan — [3]Department of Physics, Purdue University, USA — [4]Materials Science Centre, Indian Institute of Technology, India

Stacked transition metal dichalcogenide monolayers are emerging as a platform to study correlated phases such as Mott insulators or Wigner crystallization. Spatially resolved ARPES can potentially visualize the moiré bands and hybridization effects in the electronic structure underpinning these correlated phases. Observing these phenomena in ARPES in a reproducible way remains challenging, motivating systematic studies of interlayer interactions in twisted TMD bilayers. 20 different heterobilayers of WSe_2, WS_2, $MoSe_2$, and WS_2, as well as homobilayers of WSe_2 are fabricated with varying twist angles. Their electronic properties are measured using the microARPES branch at the ASTRID2 synchrotron at Aarhus University. Band alignments and hybridization effects are tracked as a function of material composition and twist angle. The used dry-transfer fabrication techniques do not yield the direct observation of flat bands from moiré effects in the valence band. Based on this work future avenues for reproducibly attaining moiré effects in photoemission from TMDs are discussed.

HL 50.2 Thu 15:15 H6

Gate-Tunable miniband dispersion in twisted graphene superlattices near the magic angle measured with MicroARPES — •Alfred J. H. Jones[1], Zhihao Jiang[1], Dongkyu Lee[2], Youngji Park[2], Kimberly Hsieh[1], Paulina Majchrzak[1], Chakradhar Sahoo[1], Thomas S. Nielsen[1], Kenji Watanabe[3], Takashi Taniguchi[3], Philip Hofmann[1], Jill A. Miwa[1], Yong P. Chen[1,4], Jeil Jung[2], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, University of Seoul, Korea — [3]National Institute for Materials Science, Japan — [4]Department of Physics and Astronomy, Purdue University, USA

Twisted superlattices of mono- and bilayer-graphene are emerging as powerful tools to explore quantum many-body effects such as unconventional superconductivity and Mott insulating states. Access to the momentum-resolved electronic structure simultaneous to changing the carrier concentration and displacement field within a twisted superlattice device can directly provide key information on the miniband dispersion tunability that underpins the correlated phenomena.

Here, we present microARPES measurements from SGM4 at ASTRID2 on two-terminal "near-magic-angle" twisted bilayer (TBG) and double-bilayer graphene (TDBG) devices. Our findings for the two systems are strikingly different: On TBG, we find a filling factor-dependent bandwidth change of the flat moiré bands, whereas on TDBG the effect of tuning the doping and displacement field leads to non-monotonous bandwidth changes and tunable gap opening effects.

HL 50.3 Thu 15:30 H6

Topological magnetic Moiré heterostructures — •Aymeric Saunot[1,3], Sebastien E. Hadjadj[2], Tonica Valla[1], Maxim Ilyn[3], and Ilya I. Klimovskikh[1] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastían, Basque Country, Spain. — [2]Materials Physics Center (MPC), Paseo Manuel de Lardizabal N5,b20018 Donostia, Spain. — [3]Departamento de Física de Materiales UPV/EHU, San Sebastían, Spain.

Over the last few years Moiré superlattices have become a hot topic in condensed matter, thanks to the experimental success of magic angle twisted graphene. Moiré superpotentials arise from either twist or atomic mismatch at the interface between van der Waals materials, leading to a rich physics of strongly correlated electrons. Intriguingly, creation of Moiré pattern on the surface of 3D topological insulator (TIs) is theoretically expected to lead to, among others, topological superconductivity, high Chern number systems and non-trivial magnetic textures. Here, we present Moiré heterostructures made from 3D TIs and novel 2D magnetic insulators transition metal dihalides. We investigate the heterostructure's surface by means of STM, ARPES, XMCD, and LEED. Our results show that the Moiré periodicity and the symmetry of the potential, can be tuned based on the ratio between the lattice parameters of the heterostructure's layers. Band structure measurements excitedly show the main Dirac cone surrounded by several Dirac cone replicas creating new Dirac minicones at the crossing points, opening a whole new platform to study topological Moiré physics.

HL 50.4 Thu 15:45 H6

SNOM of lateral TMDC heterojunctions — •Philipp Schwendke[1], Samuel Palato[1], and Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG

Two transition metal dichalcogenide monolayers, joined together laterally, form a one-dimensional heterojunction where charge transfer with associated space charge region and current rectification have been shown experimentally [1]. Furthermore, there are unique local electronic properties determining the excitonic response in the boundary region. Nanoscale spectroscopic methods are needed for the observation of such local optical properties. We use scanning near-field optical microscopy (SNOM) in combination with a continuous wave (cw) light source at 633 nm, as well as a pulsed laser tunable in a wide range from 250 nm to 1300 nm. We employ pseudo-heterodyne modulation for noise suppression and optical phase information, and quadrature-assisted discrete demodulation in order to use the tunable light source at kHz repetition rates. Resonant SNOM measurements show a quenching near the WS_2-MoS_2 boundary, which can be indicative of local energy shifts or electronic states specific to the boundary region. This is complementary to previous measurements which show quenching of photoluminescence [2], attributing it to exciton recombination. In addition, the agreement of results acquired with cw and pulsed light sources paves the way towards time-resolved near-field measurements.

[1] Li et al., Science, vol 349, p 524 (2015)
[2] Chou et al., Nanoscale, vol 14, p 6323 (2022)

HL 50.5 Thu 16:00 H6

Charge density wave interactions in bilayer 1T-TaSe2 — •Robert Drost, Ziying Wang, Büşra Arslan, Adolfo Fumega, Jose Lado, and Peter Liljeroth — Aalto University, Department of Applied Physics

Van der Waals materials offer splendid opportunities for quantum material engineering through stacking and heterostructure formation. While well-proven for many essential two-dimensional materials, these techniques are less explored for correlated materials. The 1T phase of TaSe2 is a two-dimensional Mott insulator and and excellent model system for correlations in reduced dimensions. The correlation gap in 1T-TaSe2 is highly sensitive to the thickness of the material, suggesting that electron-electron interactions between the charge density waves play an important role in determining the electronic properties of few-layer TaSe2. We also observe and additional site dependence of the gap size, showing that the stacking order may be equally important. These effects hint at the possibility of using charge density wave stacking as a design element in new quantum materials.

HL 50.6 Thu 16:15 H6

Giant Zeeman effect at a magnetic topological van der Waals interface — Tobias Wichmann[1,2], Keda Jin[1,3], Jose Martinez-Castro[1,3], Tom G. Saunderson[4,5], Honey Boban[6], Lukasz Plucinski[6], Yuriy Mokrousov[4,5], Markus Ternes[1,3], F. Stefan Tautz[1,2], and •Felix Lüpke[1,7] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]Institut für Experimentalphysik IV A, RWTH Aachen University — [3]Institut für Experimentalphysik II B, RWTH Aachen University — [4]Institute of Physics, Johannes Gutenberg University Mainz — [5]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich — [6]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [7]II. Physikalisches Institut, Universität zu Köln

We report giant Zeeman effects with Landé g-factors up to $g \approx 230$ at the interface of graphene and the van der Waals (vdW) ferromagnet Fe_3GeTe_2 (FGT). They arise from orbital moments generated by the non-trivial band topology of the FGT and cause a huge asym-

metric level splitting when a magnetic field is applied. By exploiting the inelastic phonon gap of graphene, we can directly access the vdW interface to the FGT underneath by scanning tunnelling microscopy and spectroscopy. By analyzing the Faraday-like screening of the tunnelling tip by the graphene, we are able to quantify the electric field at the vdW interface.

HL 50.7 Thu 16:30 H6

Nanoscale band-gap modulation and dual moiré superlattices in the weakly-coupled h-BN/graphite heterostructure — Fábio J. R. Costa[1,2], Luiz F. Zagonel[1], Tin S. Cheng[3], Jonathan Bradford[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergei V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Klaus Kuhnke[2], Klaus Kern[2,6], and •Anna Rosławska[2] — [1]Unversity of Campinas, Brazil — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Nottingham, United Kingdom — [4]Laboratoire Charles Coulomb, Montpellier, France — [5]Institut Universitaire de France, Paris, France — [6]EPFL, Lausanne, Switzerland

Van der Waals materials, such as hexagonal boron nitride (h-BN), and their heterostructures are highly promising for novel nanophotonic and electronic devices. In such stacks, moiré patterns arise and modulate the electronic properties of the material at the scale of typical superstructure periods (approx. 10 nm), and as such are challenging to probe. Here, we investigate the moiré superlattices in the weakly coupled h-BN/graphite heterostructure at the atomic scale. Scanning tunneling microscopy (STM) imaging reveals extensive moiré unit cells on the surface, while spectroscopic measurements demonstrate significant modulation in the work function and band gap across the periodic supercell. Additionally, we identify a dual moiré superlattice in twisted bilayers of h-BN on graphite, providing an extra degree of freedom to tune the heterostructure's properties.

HL 50.8 Thu 16:45 H6

Impact of point defects and grain boundaries on sulfur diffusion and memristive properties of MoS_2 single sheets — •Aaron Flötotto[1], Jules Oumard[1], Benjamin Spetzler[2], Martin Ziegler[2], Erich Runge[1], and Christian Dressler[1] — [1]Technische Universität Ilmenau, Germany — [2]Christian-Albrechts-Universität zu Kiel, Germany

The memristive properties of transition metal dichalcogenides, such as MoS_2, are currently the subject of intense research and have recently been traced back to the dynamics of sulfur vacancies [1, 2]. In this theoretical work, we employ molecular dynamics to determine the sulfur vacancy diffusion coefficients in the vicinity of various point defect structures and grain boundaries in single sheet MoS_2. To address the necessity of large cell sizes and long time scales, we utilize machine learning force fields, applying both Gaussian approximation potential and equivariant graph neural networks. We then compare the accuracy of these force fields and discuss the results in regard to the memristive properties of MoS_2. Our findings indicate a reduction in energy barriers for sulfur vacancy diffusion as the size of vacancy clusters increases and highlight the importance of certain interstitial sites in these vacancy clusters.

[1] Li, D., et al. (2018). ACS Nano, 12(9), 9240-9252. doi.org/10.1021/acsnano.8b03977

[2] Spetzler, B., et al. (2024). Adv. Electron. Mater., 10, 2300635. doi.org/10.1002/aelm.202300635

HL 50.9 Thu 17:00 H6

Machine-Learning the Electronic Structure of Twisted Bilayer Graphene — •Lenz Fiedler[1], Agnieszka Kuc[1], Florian Arnold[2], and Attila Cangi[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Dresden, Deutschland — [2]Technische Universität Dresden, Dresden, Deutschland

Twistronics, i.e., the study of twodimensional materials in which individual layers are twisted w.r.t.õne another, has the potential to significantly propel technological progress. Twisted bilayer materials, e.g., graphene, may exhibit a significant change in electronic structure and electrical properties based on twist angle. Their computational treatment with density functional theory (DFT) proves difficult, as small twist angles affect the periodicity of the cell and can only be simulated with large unit cells. In this talk, the recently introduced Materials Learning Algorithms (MALA) - a framework for accelerating DFT calculations based on machine learning - is applied to twisted bilayer graphene. Bilayer graphene serves as a proxy for the larger field of twistronics itself. It is shown how the electronic structure, including electronic density of states and electronic charge density, can be predicted from a small number of twist angles for a range of twisted bilayer graphene structures. Since the MALA framework uses the local density of states to encode the electronic structure on a numerical grid, predictions can be made on much larger length scales than with standard DFT calculations. This work demonstrates how machine learning can be used to computationally model twisted bilayer structures where standard first-principles methods are not viable.

HL 50.10 Thu 17:15 H6

High-throughput *ab initio* screening of 2D heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], Roman Kempt[1], and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Heterostructure interfaces produced by stacking two-dimensional (2D) materials facilitate the development of advanced electronic functionalities down to the atomic level. The efficient autonomous creation and computational study of these systems is, however, a challenge due to the general incommensurability of the 2D monolayers. This often results in large unit cells with hundreds to thousands of atoms.

Here, we present an extensive *ab initio* screening of heterostructures made of 2D systems. The approach makes use of the AFLOW-Hetbuilder – a newly developed tool that automates the heterotructure generation based on coincidence lattice theory [1,2]. It is fully integrated into the AFLOW framework [3,4]. We study the binding energy of a large set of heterostructures and also analyse their structural, electronic, and magnetic properties [5]. The presented efficient workflow can enable the systematic data-driven design of 2D heterostructures.

[1] D. S. Koda *et al.*, J. Phys. Chem. C **120**, 10895 (2016).
[2] https://zenodo.org/record/4721346.
[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[4] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[5] A. Nihei *et al.*, manuscript in preparation (2024).

HL 50.11 Thu 17:30 H6

Size-Dependent Diffusion of Radioactive Alcohols Through CNMs — •Neita Khayya, Andre Beyer, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Conventional membranes frequently struggle to achieve both, high permeance and high selectivity. On the other hand, two-dimensional membranes demonstrated remarkable progress. For example, nanometer-thin carbon nanomembranes (CNMs) from self-assembled monolayers of terphenylthiol molecules combine rapid water permeation with a rejection of ethanol in pressure-driven experiments as well as ultrahigh ionic exclusion in ion conductivity measurements. Although there has been great progress in understanding the distinctive characteristics of CNMs, more work is required to fully understand their transport characteristics, which requires complementary approaches. In this work, we employed the radio-active tracer diffusion method to study the size-depended concentration-driven permeation of different alcohols, namely [14C] CnH2n+1OH (n = 1*3) through thickness-varied CNMs from biphenylthiol (BPT), terphenylthiol (TPT) as well as quaterphenylthiol (QPT) molecules. Our findings align with vaporous alcohol pressure-driven permeation measurements regarding the size exclusion through CNMs. Interestingly, our results indicate an increased permeation rate in the liquid phase, which can be rationalized by hydrogen bonds created inside the membrane between the water molecules and diffused alcohols.