O 83: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

O 83.1 Thu 10:30 H11

Charge ordered phases in the hole-doped triangular Mott insulator 4*Hb*-TaS_2 — •Byeongin Lee[1], Junho Bang[1], Hyungryul Yang[1], Sunghun Kim[2], Dirk Wulferding[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, Ajou University, Suwon 16499, Republic of Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Republic of Korea

4*Hb*-TaS_2 has a unique layered structure, featuring a heterojunction between a 2D triangular Mott insulator and a charge density wave metal. Since a frustrated spin state in the correlated insulating layer is susceptible to charge ordering with carrier doping, it is required to investigate the charge distribution driven by interlayer charge transfer to understand its various phases. In this study, we utilize scanning tunneling microscopy and spectroscopy (STM/S) to examine the charge-ordered phases of 1 *T*-TaS_2 layers within 4*Hb*-TaS_2, explicitly focusing on the non-half-filled regime. Our STS findings reveal an energy gap that exhibits an out-of-phase relation of the charge density. We attribute the emergence of the charge-ordered insulating phase in a doped triangular Mott insulator to the interplay between on-site and nonlocal Coulomb repulsion.

O 83.2 Thu 10:45 H11

Superlattice engineering in graphene and 1T-$NbSe_2$ heterostructures — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I. Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering has become a major branch of condensed matter research, not at least due to the variety of exotic states observed twisted in van der Waals heterostructures. We here present a new method to periodically modulate graphene by stacking it on 1T/2H-$NbSe_2$. By tuning the twist angle, we realized two near-commensurate superlattices: $\sqrt{3}\times\sqrt{3}$ and 2×2 aligned with the charge density wave (CDW) of 1T-$NbSe_2$. Using scanning tunnelling microscopy, we visualized local stacking configurations for these two superlattices. We applied a newly developed symmetry analysis method to track rotational symmetry breaking as a function of bias. In the 2×2 superlattice, C_3 rotational symmetry was preserved. However, in the $\sqrt{3}\times\sqrt{3}$, a strong strip phase occurs. This symmetry breaking is explained by our tight-binding model. Our findings highlight a mechanism for superlattice-induced symmetry breaking that hints towards exotic states of matter.

O 83.3 Thu 11:00 H11

Influence of Edge Termination on the Electronic Structure of Single Layer MoS_2 on Graphene/Ir(111) — •Alice Bremerich[1], Marco Thaler[2], Thais Chagas[1], Borna Pielic[1], Laerte Patera[2], and Carsten Busse[1] — [1]Universität Siegen, Deutschland — [2]Universität Innsbruck, Österreich

MoS_2 is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic edge state that induces partial charge accumulation at its edges, resulting in band bending effects. This 1D state acts as a barrier to electron transport across the edge and contributes significantly to quantum confinement effects in TMDC islands. In this study, we tune the edge state and the associated band bending by altering the edge termination of MoS_2/gr/Ir(111) and investigate the resulting changes in the electronic structure by Scanning Tunneling Microscopy and Spectroscopy (STM and STS) at 8 K.

Quasi-freestanding MoS_2 is grown on gr/Ir(111) by Molecular Beam Epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). We vary the chemical potential of sulfur and thereby modify the chemical environment of the boundaries. The partial charge at the perimeter depends on edge type as well as edge chemistry. In consequence, also the upward bending of both valence and conduction band shows distinct variations.

O 83.4 Thu 11:15 H11

magnetic-field-induced dimensionality transition of charge density waves in strained 2H-NbSe2 — •Ryo Ichikawa[1], Yukiko Takahashi[2], Eiichi Inami[3], and Toyo Kazu Yamada[1,4] — [1]Department of Material Science, Chiba University — [2]National Institute for Material Science, Tsukuba — [3]School of system Engineering, Kochi University of Technology — [4]Molecular Chirality Research center, Chiba University

Layered transition metal dichalcogenides (TMDs) exhibit various correlated phases, including charge density waves (CDW), superconductivity, and magnetic orders. Bulk 2H-NbSe2 (2H niobium diselenide) is one of the most extensively studied TMDs, showing a triangular (3Q) incommensurate CDW with a 3a period in real space (3 * 3, TCDW ~ 33 K). Electric and magnetic fields have been used to manipulate spatial or time inversion symmetry, while the CDW in 2H-NbSe2 remains robust even under large magnetic fields on the order of tens of Tesla. However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe2, where a weak magnetic field of approximately 30 mT can switch the electronic phase within the thin film, resulting in a supercurrent diode effect. This study investigates the strained 2H-NbSe2 exhibiting the 2*2 CDW phase. We utilize low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) in ultra-high vacuum (UHV). STS maps reveal the coherence of the 2*2 CDW patterns. However, applying an out-of-plane magnetic field induces a dramatic transformation akin to that observed in 1T-NbSe2, shifting the metallic 2D CDW pattern to a 1D CDW pattern.

O 83.5 Thu 11:30 H11

Ultrafast phonons dynamics of monolayer transition metal dichalcogenides — •yiming pan and fabio caruso — Kiel University, Germany

Valley degrees of freedom in transition-metal dichalcogenides influence thoroughly electron-phonon coupling and its nonequilibrium dynamics. Here we present a time-resolved ab-initio study of the ultrafast dynamics of chiral phonons following carrier excitation with circularly-polarized light. By investigating the valley depolarization dynamics of monolayer MoS_2 and WS_2, we find that a population imbalance of carriers distributed at K and K′ can lead to valley polarized phonons persisting beyond 10 ps, and characterized by a distinctive chirality [1]. Additionally, we find that strain can be exploited as a tool to control the phonon emission and the relaxation channels of hot carriers [2]. Finally, we briefly discuss available opportunities for experimental detection of these phenomena

[1] Y. Pan and F. Caruso, Nano Lett. 23, 7463 (2023)
[2] Y. Pan and F. Caruso, npj 2D Mater. Appl. 8, 42 (2024)

O 83.6 Thu 11:45 H11

Probing Excitonic Properties and Structural Effects in WS_2-Graphene Heterostructures Using EELS and DFT-BSE Modeling — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Robin Günkel, Badrosadat Ojaghi Dogahe, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the excitonic properties of WS_2 epitaxially grown on graphene by metal-organic chemical vapor deposition. We focus on understanding the effects of structural changes, such as variations in the number of WS_2 layers. Using monochromatic electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), we observe in the monolayer region of WS_2 an excitonic spectrum with excitonic peaks at 2.0 eV and 2.4 eV, as well as additional spectral features at higher energies. Measurements in the bilayer region show a small redshift of these features due to the additional layer. Complementary density functional theory and Bethe-Salpeter calculations show that this redshift in the K-valley excitons is due to both a change in quantum confinement and a change in the WS_2 lattice constant, with the latter being the dominant effect. Using STEM, this lattice distortion can be attributed to the heteroepitaxial alignment of the lower WS_2 layer to the graphene substrate, while the upper layer is relaxed. This study provides valuable insights into the relationship between atomic structure and optical properties in complex material systems, providing essential knowledge for the design and optimization of 2D heterostructures for advanced device applications.

O 83.7 Thu 12:00 H11

Optical excitations in 2H-MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Münster, Institute of Physics and Center for Nanotechnology, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Theoretical and experimental investigations have shown several changes in the optical spectrum of the 2H-MoS_2 bilayer under pressure [1].

By using density functional theory (DFT) and many-body perturbation theory in combination with linear elasticity, our computational investigations show an effective shift of the A exciton under pressure. It is strongly connected to the behavior of the direct band gap at the K point, which shifts in energy under pressure. The direction of this shift depends on the stress condition. While a hydrostatic pressure leads to a blueshift, a suppression of the in-plane contraction, as it appears in diamond anvil cell-experiments due to the interaction between the sample and the substrate, shows a redshift.

Moreover, we observe a similar behavior for the interlayer exciton, whereas the shift rate is smaller than that of the A exciton, which results in a decreasing A-IL splitting for an increasing pressure.

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

O 83.8 Thu 12:15 H11

Visualizing and controlling charge states of metal nanoislands on a two dimensional semiconductor — •Junho Bang[1], Byeongin Lee[1], Jian-Feng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul, Korea — [2]Department of Topological Quantum Chemistry, Max Planck Institute for Chemical Physics of Solids, München ,Germany

Nanoscale objects show unique electronic behaviors when weakly coupled to electrodes. Coulomb blockade (CB) can occur in such systems, where the repulsive Coulomb interaction between electrons prevents additional electrons from entering the quantum dots, hindering their flow. Single electron tunneling occurs by these correlated electron transports, leading to the discrete charge states of objects in double barrier tunneling junctions. Despite enormous progress, challenges remain in precisely controlling the interplay between objects' charge states and tunneling dynamics under varying conditions. Here, we visualize the charge states and their spatial variation on the random array of the indium islands on two-dimensional semiconductor black phosphorus using scanning tunneling microscopy and spectroscopy. Our spatially resolved tunneling spectra reveal that the junction capacitance varies across the islands. Furthermore, we find that the CB features are visible outside the islands, which is attributed to the remote gating of the islands. Our work advances the manipulation of electron transport at the nanoscale, which will be helpful in the application of nanoscale object-based single-electron devices.