

TT 12: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g. via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15

Location: HSZ/0003

Topical Talk TT 12.1 Mon 15:00 HSZ/0003

Charge confinement in twisted bilayer graphene — ●CHRISTOPH STAMPFER — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Twisted bilayer graphene (tBLG) near the magic angle is a unique platform where the combination of topology and strong correlations gives rise to exotic electronic phases. These phases are gate-tunable and related to the presence of flat electronic bands, isolated by single-particle band gaps. This enables charge confinement and allows to explore the interplay of confinement, electron interactions, band renormalisation and the moiré superlattice, potentially revealing key paradigms of strong correlations. In this talk we will present two experiments where we study charge confinement in tBLG. First, we report on the observation of negative electronic compressibility in tBLG for Fermi energies close to insulating states. To observe this negative compressibility, we take advantage of naturally occurring twist-angle domains that emerge during the fabrication of the samples, leading to the formation of charge islands. Second, we present gate-defined single-electron transistors (SETs) in near-magic-angle tBLG with well-tunable Coulomb blockade resonances. These SETs allow to study magnetic field-induced quantum oscillations in the density of states of the source-drain reservoirs, providing insight into gate-tunable Fermi surfaces of tBLG and open the door to quantum dots and Josephson junction arrays in tBLG.

Topical Talk TT 12.2 Mon 15:30 HSZ/0003

Tuning Coulomb interactions and Hubbard bands in 1T-TaS₂ — ●ANNA GALLER — Institute of Theoretical and Computational Physics, TU Graz, Austria — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Monolayer 1T-TaS₂ hosts a star-of-David charge-density wave (CDW) that stabilizes a low-temperature Mott-insulating state. Recent time-resolved spectroscopies indicate a coupling between the CDW amplitude mode and the electronic correlation strength, yet the role of the screened Coulomb interaction remains unclear. Using the constrained random-phase approximation, we show that the CDW amplitude modifies the bare and screened on-site interactions, leading to sizable variations in the effective Hubbard U . Our combined density-functional and dynamical mean-field theory calculations reveal that the Hubbard bands shift in concert with the CDW amplitude, and that a reduced distortion drives a transition from a Mott insulator to a correlated metal. These results demonstrate a direct link between lattice distortions and Coulomb interactions in transition-metal dichalcogenides, providing a microscopic mechanism for light-induced control of correlated phases in two-dimensional quantum materials.

Topical Talk TT 12.3 Mon 16:00 HSZ/0003

Optical signatures of interlayer electron coherence in a bilayer semiconductor — ●NADINE LEISGANG^{1,2}, XIAOLING LIU², PAVEL DOLGIREV², PHILIP KIM², and MIKHAIL LUKIN² — ¹Phillips-Universität Marburg, Germany — ²Harvard University, United States

Emergent strongly correlated electronic phenomena in atomically thin transition-metal dichalcogenides represent an exciting frontier in con-

densed matter physics, with examples ranging from bilayer superconductivity and electronic Wigner crystals to the ongoing search for exciton condensation. Here, we take a step towards the latter by reporting experimental signatures of unconventional coupling of interlayer excitons consistent with coherence between interlayer electrons in a transition-metal dichalcogenide bilayer. We investigate naturally-grown MoS₂ homobilayers integrated in a dual-gate device structure allowing independent control of the electron density and out-of-plane electric field. When the bilayer is electron-doped under conditions where tunnelling between layers is negligible, we observe that two interlayer excitons - which normally should not interact - hybridize in a way distinct from both conventional level crossing and anti-crossing. We show that these observations can be explained by quasi-static random coupling between the excitons, which increases with electron density and decreases with temperature. We argue that this phenomenon is indicative of a spatially fluctuating order parameter in the form of interlayer electron coherence - a theoretically predicted many-body state that has yet to be unambiguously established experimentally outside the quantum Hall regime.

15 min. break

Topical Talk TT 12.4 Mon 16:45 HSZ/0003

Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures — ●AMMON FISCHER — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — Center for Computational Quantum Physics, Flatiron Institute, New York, NY 10010, USA

Moiré materials - twisted stacks of two-dimensional materials - bridge between two influential paradigms of condensed matter research: non-trivial quantum geometry and strong electron-electron interactions. In this talk, I will outline how the construction of faithful low-energy models and their successive treatment by state-of-the-art many-body techniques allows to resolve electronic order in moiré and non-moiré heterostructures from first principles. In twisted bilayers of WSe₂, functional renormalization group techniques allow to unravel the angle evolution of antiferromagnetic order and superconductivity in the crossover regime from weak-to-moderate interactions. In rhombohedral multilayer graphenes, the low-energy theory is naturally described in terms of supercell Wannier functions that span the effective $U(4) \times U(4)$ subspace of the spin, valley and layer degrees of freedom. Electronic correlations give rise to various iso-spin ordered regimes, superconductivity and charge density wave order at low electronic densities bridging to the physics of their twisted counterparts.

Topical Talk TT 12.5 Mon 17:15 HSZ/0003

Mesoscale Atomic Engineering in a Crystal Lattice — ●JULIAN KLEIN — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

Controlling the arrangement of individual atoms with lasers, ion traps, and scanning probe techniques has enabled quantum simulation and computing platforms that transcend naturally occurring configurations of matter. Yet achieving comparable atomic control within a solid and at scale remains a foundational challenge, one that could revolutionize

the design of artificial matter. Here, I demonstrate atomic engineering of artificial matter inside a scanning transmission electron microscope. By developing strategies to position and move the electron beam with few-picometer accuracy, deterministic control over atomic motion in both space and time is achieved. Full automation of the microscope enables the creation of three-dimensional defect superlattices in many-nanometer thick CrSBr with user-defined lattice spacing and symmetry, spanning tens of thousands of engineered sites over fields of view exceeding one hundred nanometers, all generated in under an hour. Our results establish atomic engineering in the electron microscope as a practical reality, opening unprecedented opportunities to create quantum defects and quantum phases with tunable charge and spin interactions, and to control host-lattice excitations by arranging atoms in patterns that are commensurate or incommensurate with the underlying crystal over mesoscopic, and potentially micro- or macroscopic, length scales.

TT 12.6 Mon 17:45 HSZ/0003

Interlayer electrodynamics of CDWs in van der Waals materials and heterostructures — ACHYUT TIWARI, RENJITH MATHEW ROY, MAXIM WENZEL, CHRISTIAN PRANGE, BRUNO GOMPF, and •MARTIN DRESSSEL — 1. Physikalisches Institut, Universität Stuttgart

Layered transition metal dichalcogenides such as 1T-TaS₂, 2H-TaS₂ and their natural heterostructure 4H_b-TaS₂ provide a platform for studying interlayer coupling, orbital hybridization, and charge transfer that determine collective electronic phenomena, such as unconventional superconductivity and strong electronic correlations. Temperature-dependent infrared measurements of the in-plane and out-of-plane optical response of 1T-TaS₂ across its CDW-driven metal-insulator transition are combined with DFT calculations. We find that a quasi-1D instability that induces interlayer dimerization is responsible for the MI-transition. Furthermore, spectroscopic ellipsometry combined with an anisotropic Bruggeman effective medium approximation reveals that metallic domains evolve in a strongly anisotropic way and often extend along the out-of-plane direction as the transition

proceeds.

When 1T-TaS₂ is stacked between 1H-TaS₂, forming a natural heterostructure of 4H_b-TaS₂, charge transfer occurs between the layers, that can be tuned with temperature, and which is related to the CDW in 1T-TaS₂ layer. We conclude that the phase transition in 1T-TaS₂ is inherently three dimensional, despite its layered structure, and that interlayer coupling is essential for its electronic structure and phase behavior both individually and in heterostructures.

TT 12.7 Mon 18:00 HSZ/0003

Enhancing Plasmonic Superconductivity in Layered Materials via Dynamical Coulomb Engineering — •YANN IN 'T VELD¹, MIKHAIL I. KATSNELSON^{2,3}, ANDREW J. MILLIS^{4,5}, and MALTE RÖSNER^{2,6} — ¹I. Institute of Theoretical Physics, Universität Hamburg, Hamburg, Germany — ²Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — ³Constructor Knowledge Institute, Constructor University, Bremen, Germany — ⁴Center for Computational Quantum Physics, Flatiron Institute, New York, United States of America — ⁵Department of Physics, Columbia University, New York, United States of America — ⁶Faculty of Physics, Bielefeld University, Bielefeld, Germany

Conventional Coulomb engineering, through controlled manipulation of the environment, offers an effective route to tune the correlation properties of atomically thin van der Waals materials via static screening. Here we present tunable *dynamical* screening as a method for precisely tailoring bosonic modes to optimize many-body properties. We show that “bosonic engineering” of plasmon modes can be used to enhance plasmon-induced superconducting critical temperatures of layered superconductors in metallic environments by up to an order of magnitude, due to the formation of interlayer hybridized plasmon modes with enhanced superconducting pairing strength. We determine optimal properties of the screening environment to maximize critical temperatures. We show how bosonic engineering can aid the search for experimental verification of plasmon mediated superconductivity.