TT 88: 2D Materials and Heterostuctures: (Twisted) Bilayers (joint session HL/TT)

Time: Friday 9:30–12:15 Location: EW 201

TT 88.1 Fri 9:30 EW 201

Lattice relaxation, electronic structure and continuum model for twisted bilayer MoTe2 — •Ning Mao[1], Cheng Xu[2,3], Jiangxu Li[2], Ting Bao[3], Peitao Liu[4], Yong Xu[3], Claudia Felser[1], Liang Fu[5], and Yang Zhang[2,6] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA — [3]Department of Physics, Tsinghua University, Beijing 100084, China — [4]Institute of Metal Research, Chinese Academy of Sciences, 110016 Shenyang, China — [5]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [6]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Our study delves into the effect of lattice relaxation on the moiré band structures of twisted bilayer MoTe2, implemented by large-scale first-principles calculations and transfer learning neural network. Throughout our study, we have incorporated two van der Waals correction methods: the Grimme D2 method and a density-dependent energy correction. Notably, the latter method demonstrates a continuous evolution of bandwidth with respect to twist angles. Our findings reveal the critical role of in-plane lattice displacements, which generate substantial pseudomagnetic fields, reaching up to 250 T. Building on these insights, we have developed a comprehensive continuum model with a single set of parameters for a wide range of twist angles, providing a useful starting point for many-body simulation.

TT 88.2 Fri 9:45 EW 201

Twist disorder in $tWSe_2$: Insights from Lateral Force Microscopy and Raman Spectroscopy — •Nicolai-Leonid Bathen[1], Rami Dana[2], Hendrik Lambers[1], Nihit Saigal[1], Julian Klein[2], Frances M. Ross[2], and Ursula Wurstbauer[1] — [1]University of Münster, Münster, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, United States

Bilayers of twisted transition metal dichalcogenides (TMDCs) form moiré hybridized lattices resulting in moiré minibands [1] which leads to the capability to host correlated quantum phases [2] and to simulate Mott-Hubbard physics [3]. These properties vary strongly with the local twist angle configuration due to changes in the moiré cell size, symmetry and long-range disorder. Here we unravel the formation of moiré lattices and local disorder in the twist angle in twisted WSe_2 homo-bilayers ($tWSe_2$) by lateral force microscopy in ambient providing atomic resolution. We studied several $tWSe_2$ bilayers with a large variety in the nominal twist angle of 3° to 11° and find a surprisingly large variation in twist angle up to 1° within less than a micrometer distance. We contrast those findings with low-frequency Raman measurements sensitive to interlayer coupling and we will discuss consequences of the local twist disorder for collective inter-moiré band excitations studied by resonant inelastic light scattering [1].

[1] N. Saigal et al., arXiv 2310 14417 (2023) [2] N. P. Wilson et al., Nature 599, 383-392 (2021) [3] S. Ryee and T. O. Wehling, Nano Lett. 23 (2), 573-579 (2023) [4] Y. Song and E. Meyer, ACS Langmuir 39, 15409 (2023)

TT 88.3 Fri 10:00 EW 201

Electrical tuning of moiré excitons in $MoSe_2$ bilayers — •Joakim Hagel[1], Samuel Brem[2], and Ermin Malic[2,1] — [1]Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden — [2]Department of Physics, Philipps University of Marburg, 35037 Marburg, Germany

Recent advances in the field of vertically stacked 2D materials have revealed a rich exciton landscape. In particular, it has been demonstrated that out-of-plane electrical fields can be used to tune the spectral position of spatially separated interlayer excitons. Other studies have shown that there is a strong hybridization of exciton states, resulting from the mixing of electronic states in both layers. However, the connection between the twist-angle dependent hybridization and field-induced energy shifts has remained in the dark. Here, we investigate on a microscopic footing the interplay of electrical and twist-angle tuning of moiré excitons in homobilayers [1,2]. We reveal distinct energy regions in PL spectra that are clearly dominated by either intralayer or interlayer excitons, or even dark excitons [1]. Consequently, we predict twist-angle-dependent critical electrical fields at which the material is being transformed from a direct into an indirect semiconductor [1]. Our work provides new microscopic insights into experimentally accessible knobs to significantly tune the moiré exciton physics in atomically thin nanomaterials.

[1] J. Hagel, S. Brem, E. Malic, 2023 2D Mater. 10 014013

[2] Tagarelli, F., Lopriore, E., Erkensten, D. et al. Nat. Photon. 17, 615-621 (2023)

TT 88.4 Fri 10:15 EW 201

Exciton-polaritons in twisted-bilayer heterostructures — •Francesco Troisi[1], Hannes Huebener[1], Angel Rubio[1,3], and Simone Latini[2] — [1]MPSD, Hamburg, Germany — [2]Department of Physics, DTU, Lyngby, Denmark — [3]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, NYC, USA

2D materials, such as TMDs, have attracted significant attention due to their unique electronic properties, such as tunable bandgap, high emission efficiency, and a strong excitonic binding allowing the formation of stable excitons at room temperature. Excitons in multilayer TMD structures are the object of great interest, as we find both inter- and intra-layer excitons, which give rise to a response at different energies. Previous works show that it is possible to tune the Moiré potential to control their localization, which influences the optical properties.

In the quest to understand and control excitons in novel environments, this study focuses on excitonic behavior for a twisted bilayer MoSe2/WSe2 heterostructure in an optical cavity. Our goal is to produce an all-optical Moiré-like exciton confinement by tuning the cavity. Optical cavities provide a promising approach to controlling material properties by coupling the electronic transitions in the material to the confined photons inside the cavity, which implies photonic and excitonic states cannot be separated. The so-called exciton-polariton states are obtained. In the strong coupling regime, one needs to go beyond the perturbative approach to treat the light-matter problem.

This study utilizes the full diagonalization of the QED problem built from the Wannier equation in k-space and the Moiré potential.

TT 88.5 Fri 10:30 EW 201

Investigating the orbital dependence of the superlattice potential in Moiré semiconductors with NanoARPES — •Gianmarco Gatti[1], Julia Issing[1], Dario Rossi[2], Louk Rademaker[2], Anna Tamai[1], and Felix Baumberger[1] — [1]Department of Quantum Matter Physics, University of Geneva, Geneva, 1211, Switzerland — [2]Department of Theoretical Physics, University of Geneva, Geneva, 1211, Switzerland

Moiré semiconductors emerged as tunable quantum simulators for strongly correlated phases. The single-particle low-energy physics is ruled by the moiré-periodic superpotential that develops by twisting or stacking layers with different lattice parameters. Signatures of this modulation are observed in the spectral function measured by angle-resolved photoemission spectroscopy (ARPES) in the form of replicas and gaps opening at the nascent zone boundary. In twisted bilayer transition metal dichalcogenides (TMDs), flat bands are reported at the Brillouin zone center and their dispersion is associated to the effective moiré potential experienced by electronic states with large out-of-plane orbital character. Here, we extend this analysis and present the orbital and wave vector dependence of this interaction over the whole Brillouin zone by comparing quantitatively our ARPES data on a TMD heterobilayer with an extended tight-binding model. Our results set the fundaments for future spectroscopic studies of the electronic correlations in moiré systems.

TT 88.6 Fri 10:45 EW 201

Confocal SHG microscopy of twisted bilayers of MoS_2 — •Nikita V. Siverin[1], Daniel J. Gillard[2], Dmitri R. Yakovlev[1], Alexander I. Tartakovskii[2], and Manfred Bayer[1] — [1]TU Dortmund, Dortmund, Germany — [2]The University of Sheffield, Sheffield, UK

We investigate the crystal and exciton symmetries in twisted MoS_2 bilayer flakes using second harmonic generation (SHG). By measuring and modeling the full dependence of the SHG signal on the linear polarization angles of incident and emitted light we reveal the underlying mechanisms of SHG. Our method employs a confocal microscopy

setup, allowing for spectroscopic investigations of different excitonic resonances.

Twisting layers of 2D materials is a familiar technique that produces a superlattice and gives rise to the phenomena called moiré structure inducing changes in optical properties.

We measured different regions of overlapping flakes: monolayer, twisted monolayers, bilayer and twisted bilayers. We observe strong SHG signal from monolayers and we can measure twisted angle by polarization anisotropies of the SHG signal. According to group theory, SHG is forbidden in bilayers, but we observe small signal with rotational anisotropy deviating from the one for monolayers.

15 min. break

Invited Talk TT 88.7 Fri 11:15 EW 201

Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene — •Anna Seiler[1], Nils Jacobsen[1], Martin Statz[1], Fabian Geisenhof[2], Felix Winterer[2], Isabell Weimer[1], Tianyi Xu[3], Zhiyu Dong[4], Leonid Levitov[4], Fan Zhang[3], and Thomas Weitz[1] — [1]University of Göttingen — [2]Ludwig-Maximilians-Universität München — [3]University of Texas at Dallas — [4]Massachusetts Institute of Technology

The bandstructure of naturally occurring Bernal bilayer graphene exhibits four linearly-dispersed Dirac cones but changes drastically when large electric displacement fields are applied across the two layers. Here, tunable van Hove singularities lead to the emergence of complex correlated states. We observe experimental signatures consistent with various interaction-driven phases, including the fractional metals of Stoner type [1, 2]. More prominently, we find competing nontrivial insulating and metallic phases at hole doping that exhibit intriguing temperature dependences and nonlinear I-V characteristics at zero magnetic fields [1]. In addition, we report a novel interaction-driven behaviour in the Stoner phases in the electron-doped regime electric-field gapped Bernal bilayer graphene [2]. Specifically, we reveal that the spin- and valley-polarized phases exhibit an insulator-like temperature dependence of the conductance that challenges the conventional picture of metallic Stoner magnetism.

[1] A. M. Seiler et al., Nature 608, 298-302 (2022)
[2] A. M. Seiler et al., arXiv:2308.00827 (2023)

TT 88.8 Fri 11:45 EW 201

Valley transport assisted by Fermi surface warping — Josep Ingla-Aynés[1], •Antonio L. R. Manesco[1], Talieh S. Ghiasi[1], Serhii Volosheniuk[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Herre S. J. van der Zant[1] — [1]Kavli Institute of Nanoscience, Delft University of Technology, Netherlands — [2]Research Center for Electronic and Optical Materials, National Institute for Materials Science, Japan — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan

Valleys are distinct energy extrema in a band structure. Graphene has a band structure with two valleys at distinct high-symmetry points. The large momentum separation of these points suppresses intervalley scattering in ballistic devices. However, even in ballistic devices, valley coherence is limited by atomically-sharp edge disorder. Gate-defined bilayer graphene devices overcome this limitation and enable the observation of valley coherent phenomena. In this work, we explored ballistic electron transport in multiterminal bilayer graphene devices. We observed specular electron-focusing between gate-defined quantum point contacts, suggesting that smooth edges preserve valley polarization. Moreover, trigonal warping of the Fermi surface causes valley-dependent electron jetting, which we detected with magnetic collimation. Our results show two current peaks in the collector signal at opposite magnetic fields, consistent with the injection of two valley-polarized electron jets. Since the valley polarization of the electron current depends on the magnetic field, collimation devices are current sources with tuneable valley polarization.

TT 88.9 Fri 12:00 EW 201

Gate screening of Coulomb interactions in Bernal bilayer graphene — •Isabell Weimer[1], Anna Seiler[1], Dong Zhao[2], Jurgen Smet[2], and R. Thomas Weitz[1] — [1]1st Institute of Physics, Faculty of Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]MPI for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Measurements on dual gated, hexagonal Boron Nitride (hBN) encapsulated Bernal bilayer graphene samples, have revealed a complex phase space for Bernal bilayer graphene, including numerous Stoner metals, a correlated insulator consistent with a Wigner-Hall crystal [1] and superconducting behavior [2].

We have investigated the influence of the gate induced Coulomb interaction screening [3] on the appearance of previously reported correlated phases in gated Bernal bilayer graphene devices, using the thickness of the dielectric hBN spacing layers as variable parameter. In direct comparison of devices studied here, which are characterized by a comparably thin h-BN layer, with the data of Seiler et. al. , we observed behavior, which is supportive of an effectively lowered magnitude of Coulomb interactions. Additionally, three features in the transport data were identified, which could potentially be indicative of phases, not reported in [1] and [2].

References: [1] Seiler, Anna M., et al. Nature 608.7922 (2022): 298-302. [2] Zhou, Haoxin, et al. Science 375.6582 (2022): 774-778. [3] Kim, Minsoo, et al. Nature communications 11.1 (2020): 2339.