TT 39: Twisted Materials / Systems (joint session TT/HL)

Time: Wednesday 17:00–18:30 Location: H31

TT 39.1 Wed 17:00 H31

Formation, persistence and ordering of local moments in magic angle twisted bilayer graphene — •Lorenzo Crippa[1,2], Gautam Rai[1], Dumitru Călugăru[3,13], Haoyu Hu[4], Luca de' Medici[5], Antoine Georges[6,7,8,9], Bogdan Andrei Bernevig[3,4,10], Roser Valentí[11], Giorgio Sangiovanni[2], and Tim Wehling[1,12] — [1]University of Hamburg — [2]University of Würzburg — [3]Princeton University — [4]DIPC, Donostia-San Sebastian — [5]ESPCI, Paris — [6]Collège de France, Paris — [7]Flatiron Institute, New York — [8]École Polytechnique, Palaiseau Cedex — [9]Université de Genève — [10]IKERBASQUE, Bilbao — [11]Goethe University Frankfurt — [12]Hamburg CUI — [13]University of Oxford

The physics of magic angle twisted bilayer graphene (MATBLG) is remarkably diverse across a wide range of dopings and temperatures.

By means of a Dynamical Mean-Field Theory (DMFT) approach, we study the effect of electronic correlations in MATBLG, with particular focus on the physics of local spin and valley isospin moments. We analyze their magnitude and screening across a broad temperature range, discuss the limits of very low and infinite temperature, and obtain two different scales for their formation (around 100 K) and ordering (around 10 K).

We discuss their implications in terms of transport properties of the system (e.g. resistivity) and of spectral features (resonance peaks) and contextualize our findings with recent experimental results.

TT 39.2 Wed 17:15 H31

Nematic versus Kekulé phases in twisted bilayer graphene under hydrostatic pressure — Miguel Sánchez Sánchez[1], Israel Díaz[1], José González[2], and •Tobias Stauber[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC — [2]Instituto de Ciencia de Materiales, CSIC

We address the precise determination of the phase diagram of magic angle twisted bilayer graphene under hydrostatic pressure within a self-consistent Hartree-Fock method in real space, including all the remote bands of the system. We further present a novel algorithm that maps the full real-space density matrix to a 4x4 density matrix based on a SU(4) symmetry of sublattice and valley degrees of freedom. We find a quantum critical point between a nematic and a Kekulé phase, and show also that our microscopic approach displays a strong particle-hole asymmetry in the weak coupling regime. We arrive then at the prediction that the superconductivity should be Ising-like in the hole-doped nematic regime, with spin-valley locking, and spin-triplet in the electron-doped regime [1].

[1] M. Sánchez Sánchez, I. Díaz, J. González, T. Stauber, Phys. Rev. Lett. (in press), arXiv:2403.03140.

TT 39.3 Wed 17:30 H31

Quantum diffusion in sheared bilayer graphene — •Taher Rhouma[1], Florie Mesple[2], Vincent Renard[3], and Guy Trambly de Laissardière[1] — [1]LPTM, CY Cergy Paris Univ., CNRS, Cergy-Pontoise, France. — [2]Dept. Physics, Univ. of Washington, USA — [3]CEA, Univ. Grenoble Alpes, IRIG, PHELIQS, Grenoble, France

The identification of correlated insulators and superconductivity in magic-angle twisted bilayer graphene (MATBG) has sparked significant interest in its electronic properties [1]. When examining the MATBG moiré patterns along the line with alternating regions of AA, AB, and BA, we observe striking similarities to those found in a 1D moiré of a sheared bilayer graphene, where one layer is laterally displaced. That may lead to a localization of the electronic states [2]. In this study, we investigate numerically the electronic and quantum transport properties in sheared bilayer graphene, focusing on how the degree of shear influences these characteristics.

[1] Y. Cao, et al., Nature **556**, 43 (2018); Nature **556**, 80 (2018).
[2] J. Gonzalez, Phys. Rev. B **94**, 165401 (2016).

TT 39.4 Wed 17:45 H31

Ab-initio fRG study on $tWSe_2$ — •Hannes Braun — Max Planck Institut für Festkörperforschung — Technische Universität München

The recent experimental reports on superconductivity in twisted WSe_2 have served to justify the already considerable interest in twisted TMD systems. From a theoretical standpoint, there have been numerous attempts to describe these systems. To study the phase diagram and analyse the governing physics, we employ the functional renormalisation group method. This approach allows us to gain an unbiased understanding of the interplay between fluctuations leading to symmetry-broken phases. To develop a model capable of describing the material, we integrate *ab-initio* results as initial conditions. In this talk, we present method developments for a more efficient momentum integration and results on the interplay between magnet and pairing instabilities.

TT 39.5 Wed 18:00 H31

Mott transitions and doping asymmetry in twisted bilayer WSe_2 — •Siheon Ryee[1], Lennart Klebl[2,1], Valentin Crépel[3], Ammon Fischer[4], Lede Xian[5,6], Angel Rubio[6,3], Dante Kennes[4,6], Andrew Millis[3,7], Antoine Georges[8,3], Roser Valentí[9], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany — [3]Flatiron Institute, New York, USA — [4]RWTH Aachen University, Aachen, Germany — [5]Tsientang Institute for Advanced Study, Zhejiang, China — [6]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [7]Columbia University, New York, USA — [8]Collège de France, Paris, France — [9]Goethe Universität Frankfurt, Frankfurt am Main, Germany

The recent discovery of superconductivity in twisted bilayer WSe_2 ($tWSe_2$) at two distinct twist angles (3.65 deg and 5 deg) along with previous reports of metal-insulator transitions, spin density wave states, and fractional Chern insulators raises deep questions in correlated electron physics. We present results of a dynamical mean-field theory-based investigation of a model that faithfully captures the band structure and topology of twisted transition metal dichalcogenides as functions of twist angle and displacement field. We find good agreement with several key aspects of the experimental data. Focusing further on the twist angle of 3.65 deg, we discuss the nature of the electric-field-induced metal-insulator transition, the experimentally observed coherence temperature, and the origin of the observed doping asymmetry in resistivity.

TT 39.6 Wed 18:15 H31

Twisted bilayer MoS_2 under electric fields: A system with tunable symmetry — •Aitor Garcia-Ruiz[1,2] and Ming-Hao Liu[1] — [1]National Cheng Kung University, Tainan, Taiwan — [2]National Graphene Institute, University of Manchester, Manchester, United Kingdom

Gate voltages take full advantage of two-dimensional systems, making it possible to explore novel states of matter by controlling their electron concentration or applying perpendicular electric fields. Here, we study the electronic properties of small-angle twisted bilayer MoS_2 under a strong electric field. We show that the transport across one of its constituent layers can be effectively regarded as a two-dimensional electron gas under a nanoscale potential. We find that the band structure of such system reconstructs following two fundamentally different symmetries depending on the orientation of the external electric field, namely, hexagonal or honeycomb. By studying this system under magnetic fields, we demonstrate that this duality not only translates into two different transport responses, but also results in having two different Hofstadter's spectra. Our work opens up a new route for the creation of controllable artificial superlattices in van der Waals heterostructures.