Electron and lattice correlations in moiré superlattices

An *ab initio* multi-scale approach to interacting electronic structure in transition metal dichalcogenide [hetero]structures

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In Short

- study of exotic quantum phases from material realistic calculations with special focus on superconducting states
- precise construction of *ab initio* based models
- incorporation of multiple tuning parameters

Over a century ago, solid state physicists came to realise that a variety of attractive and repulsive forces influence the formation of periodic structures in condensed matter. In recent years materials like graphene and hexagonal boron nitride (hBN) gained considerable interest, where especially graphene is well known as a bulk material from graphite pencils. In two spacial directions the carbon atoms in graphite are arranged in an honeycomb structure and fixed via electron binding, the third spacial direction however connects honeycomb sheets via van-der-Waals binding. Besides graphene and hBN, there is a large family of similarly structured compounds—transition metal dichalcogenides. Although one sheet of WSe_2, for instance, shows some spacial structure along the third dimension, individual layers are coupled via van-der-Waals forces. There is by now a considerable amount of work done on the investigation of such van-der-Waals materials both on the experimental and theoretical side.

Transition metal dichalcogenide bilayers host electron correlation effects like superconductivity, exciton condensation, and Mott insulation. These phenomena are adjustable via charge doping, optical excitation, dielectric environment, and twist angle [1,2].

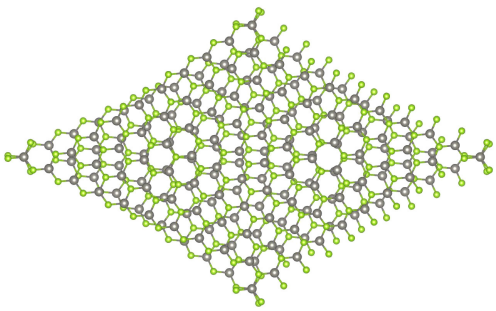

Figure 1: *Top view of moiré structure formation in tungsten diselenide bilayers upon twisting two layers with respect to each other; grey balls represent tungsten atoms, green balls selenium*

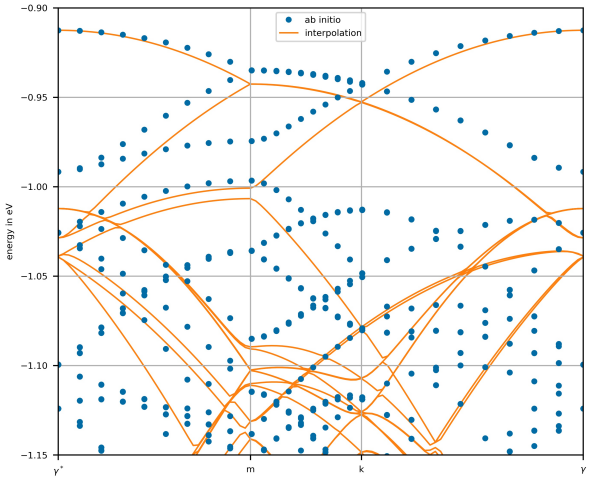

Figure 2: *Electronic bands of twisted WSe_2 at approx. 5°, constant interlayer distance and without spin-orbit coupling; results of our interpolation technique are benchmarked against large-scale DFT calculations performed in VASP, deviations in the top valence band are below 10 meV*

The complex interplay of Coulomb and electron-phonon interactions with multi-orbital and multi-valley physics behind the aforementioned correlation effects remains to be understood.

We aim to understand these phenomena in twisted structures. Fortuitously, bilayers of twisted transition metal dichalcogenides (tTMDCs) form—for certain twist angles—periodic moiré (French for marbled) structures as depicted in figure 1. This periodicity reduces the overall problem from infinitely large structures to comparably smaller, yet still large, moiré cells [3]. To build a suitable model, enabling us to investigate in which parameter regimes correlation effects occur, many-body quantum lattice models are constructed. These will encapsulate the electronic and phononic degrees of freedom as well as their coupling.

Electronic degrees of freedom are described by exploiting local negligibility of twisting. This allows for *ab initio* DFT calculations with subsequent construction of localised Wannier orbitals on untwisted snapshots of commensurate bilayers. With an automated interpolation we are able to address twisted systems (see fig. 2). The model of lattice vibrations is established by DFPT calculations, once again building upon analysis of lattice vibrations in local snapshots and interpolating to twisted systems. On this basis, we will study the impact of electron-phonon coupling on lattice stability and dynamics via calcu-

lations of phonon self-energies and investigate possible phonon-driven superconductivity within Migdal-Eliashberg theory [4].

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https://www.physik.uni-hamburg.de/en/th1.html

More Information

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[3] Carr, S., Fang, S. and Kaxiras, E. Electronic-structure methods for twisted moiré layers. Nat Rev Mater 5, 748–763 (2020). doi:10.1038/s41578-020-0214-0

[4] Giustino, F., Cohen, M.L., and Louie, S.G. Electron-phonon interaction using Wannier functions. Phys. Rev. B 76, 165108 (2007). doi:10.1103/PhysRevB.76.165108

Project Partners

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