Novel exotic states in twisted bilayer materials

Interactions in twisted superlattice quantum materials

J.M. Pizarro, C. Steinke, J. Berges, T.O. Wehling, *Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen*

In Short

- Investigation of novel exotic states in TMDC bilayer systems
- Strong correlations and Dirac physics in Star-of-David CDW bilayer TMDCs: $TaSe_2$.
- Influence of twist angles and stacking on electronic correlation phenomena

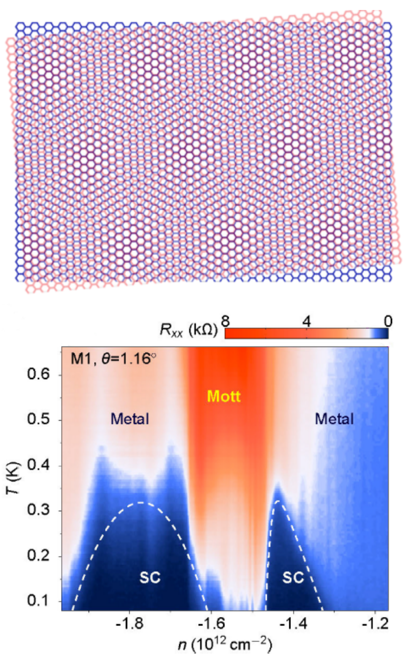

Figure 1: *(a) Twisted bilayer graphene superlattice and (b) doping-dependent phase diagram when the twist angle is $\theta = 1.16^o$, adapted from [4]. In this phase diagram, various correlated phases (e.g. Mott insulator and superconductivity) can be seen.*

Condensed matter quantum many-body states are often highly sensitive to stimuli such as pressure, temperature, or changes in chemical composition. Therefore, the concurrence of pronounced many-body phenomena in (quasi-) two-dimensional (2D) materials, with advances in synthesis and vertical heterostructuring, has fueled hopes for controlling electronic quantum phases on demand. These hopes are supported by experiments revealing electronic phase diagrams of several 2D systems - including Fe-based superconductors and transition metal dichalcogenides (TMDCs) - to be strongly dependent on dimensionality, thickness, and substrate. Most notably, recent experiments [1] on so-called twisted bilayer graphene (tBLG), see Fig. 1, have demonstrated that the absence of epitaxial constraints brings a highly effective means for materials manipulation into play: the relative twist angle between the layers θ.

Around certain *magic angles*, twisted bilayer graphene features an intricate emergent low-energy electronic structure with very flat electronic bands around the charge neutrality point, which facilitates strong correlation effects. Recent experiments [1] reported the emergence of possibly unconventional superconducting and unexpected insulating states in magic-angle tBLG at different levels of doping. The electronic states in magic angle tBLG turned out to resemble the phase diagram of high-T_c cuprate superconductors and other unconventional superconductors. While these observations created a real "hype" around correlations phenomena in tBLG, it is clear that the concept of controlling many body phenomena in van der Waals heterostructures by twisting and superlattice effects is much broader than twisted bilayer graphene.

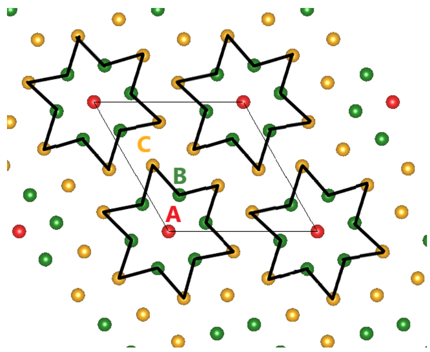

Figure 2: *Star-of-David CDW triangular superlattice of a given TMDCs. Central atom A, inner atoms B and outer atoms C can be seen forming each Star-of-David.*

The broader purpose of this project is to explore to which extent TMDC bilayer systems can realize possibly novel exotic states of quantum matter such as strongly correlated Dirac fermions. In the first year of this project, we will focus on the Star-of-David charge density wave (CDW) ordered compound 1T-$TaSe_2$, see Fig. 2. Motivated by recent experiments on bilayer 1T-$TaSe_2$ [2], our goal is to study which kind of electronic states can be realized in this system by exploiting the twisting and relative displacements between upper and lower layer as turning knobs.

Our initial goal is to explore the electronic structure of bilayer 1T-$TaSe_2$ in various stacking and twisting arrangements. To this end, we will have to perform GW-quasiparticle calculations of band structures and calculations of Coulomb matrix elements in the random phase approximation (RPA) [3,4] to asses the strength and type of electronic correlation phenomena taking place in different realizations of bilayer 1T-$TaSe_2$. The experiments from Ref. [2] indeed suggest that the ratio of the interaction strength to quasiparticle bandwidth is likely in the most interesting intermediate coupling region, but the situation is highly unclear from the theory point of view and stacking / twisting effects in the bilayer remained completely unexplored. Our goal is to change that situation during the first year of this "HLRN Großprojekt"

WWW

http://www.itp.uni-bremen.de/ag-wehling/

More Information

[1] Y. Cao et al., *Nature* **556**, 43 (2018). doi: https://www.nature.com/articles/nature26160

[2] Y. Chen et al., *arXiV* 1904.11010 (2019). doi: https://arxiv.org/abs/1904.11010

[3] C. Steinke, *PhD thesis*, Universität Bremen (2019). doi:https://elib.suub.uni-bremen.de/peid/D00107379.html

[4] J.M. Pizarro et al., *arXiv* 1904.11765 (2019). doi:https://arxiv.org/abs/1904.11765

Funding

DFG Graduiertenkolleg (GRK) (DFG-RTG 2247)