Electronic structure modelling of moiré cells in transition metal dichalcogenide heterobilayers

Bachelor or Master project in the group for computational condensed matter theory – Prof. Wehling

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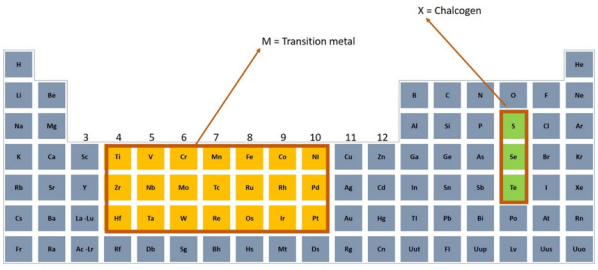
System

In this thesis project you will investigate the material class of transition metal dichalcogenides (TMDCs), i.e. combination of metallic elements from the centre of the PSE and oxygen-like elements. Similar to graphene these TMDCs form structures of hexagonal lattices. Wherefore, they are considered as so called van-der-Waals materials.

In a stacked system, for instance bilayers, it is possible to change a number of parameters: twist angle of, electron doping and materials. It is suspected that via such changes it is possible to reach novel states of correlated electrons like superconductivity or Mott physics. This project is set to tackle the heterobilayer of molybdenum disulfide and tungsten diselenide: MoS_2-WSe_2



Methodology

By twisting a bilayer system of TMDCs one looses the short range periodicity of a hexagonal lattice as the alignement is lost. For small twist angles it is possible to approximate the local misalignment of the two layers as irrelevant except for a displacement. Therefore, ab initio calculations of aligned, displaced bilayers can be used to build local tight-binding models. This includes the identification of orbital character in physically relevant electronic bands of DFT band structures in various displacements, the construction of tight-binding models via a wannierisation of the chosen band subspace, an analysis of the hopping matrix elements with respect to displacement and the construction of the moiré cell tight-binding.

Learning outcome and requirements

During the project you will learn about *density functional theory*, *Wannier orbitals* and *tight-binding* for electronic structure modelling. Additionally, the project will train you in the *usage of high-performance computing facilities* (Physnet and HLRN) as well as *programming in context of data processing and visualisation*. There are no must-have requirements for this project. Yet, having a good understanding of *quantum mechanics* and a basic understanding of *condensed matter physics* will surely be helpful.

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