ARL/Master Thesis

in the group of *Theory of Magnetic Materials*

TECHNISCHE UNIVERSITÄT DARMSTADT

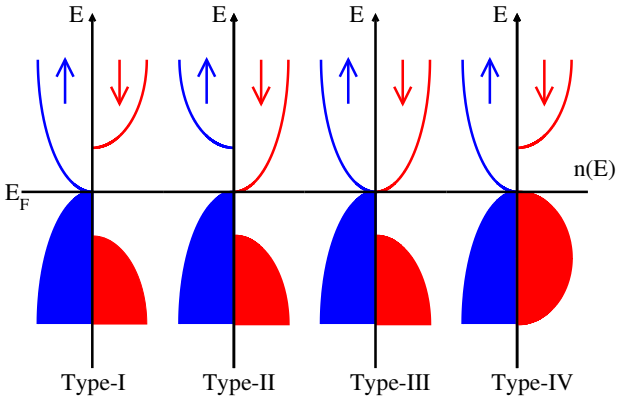
High throughput screening for 3D and 2D spin-gapless semiconductors

Spin-gapless semiconductors (SGSs) have drawn intensive attention to the spintronics community. Basically, SGSs are half metals with the majority spin channel being semimetallic, *i.e.*, the gap is zero, while there is a finite band gap in the minority spin channel. As sketched in the figure below, there are four types of SGSs, based on what are the spin characters of valence band maximum (VBM) and conduction band mimimum (CBM) and how do they touch the Fermi level, Interestingly, the VBM and CBM can touch each other at the same or different k-points, corresponding to the direct or indirect zero band gap. Whether a band gap can be opened for the direct touching cases is a fundamentally fascinating problem.

Recently, we have performed high throughput screening for 3D SGSs in quaternary Heusler compounds [1]. Further systematic calculations on more compounds with the Heusler or other structures will be done for the planned ARL/Master thesis, followed by transport and topological characterization, surface and interface effects. The expertise obtained by the prospective students are but not limited to:

1. proficiency in linux, python, and DFT.
2. capability of performing high throughput calculations using supercomputers
3. hands-on experience with the calculation of spintronic and topological properties

At least one publication is expected after completing the thesis. Please send a message to J. Prof. Hongbin Zhang (hzhang@tmm.tu-darmstadt.de) for an appointment.



Referecence

[1] Q. Gao, I. Opahle, and H. Zhang, High throughput screening for spin-gapless semiconductors in quaternary Heusler compounds arXiv:1808.02684, Phys. Rev. Mat. *accepted* (2019)