ARL/Master Thesis

in the group of *Theory of Magnetic Materials* (FB11)

TECHNISCHE UNIVERSITÄT DARMSTADT

High throughput design of 2D functional van der Waals Materials

Two dimensional materials are particularly interesting for being integrated into energy-efficient electronic devices. Motivated by the discovery of graphene in 2004, there have been tremendous progresses in developing new 2D materials, such as transition metal dichalcogenides, stanene, phosphorene, MXene, etc. Particularly, based on explicit calculations of the exfoliation energies for all materials in the ICSD database, it is predicted that 826 2D materials can be obtained (*https://materialsweb.org/twodmaterials*). We did high throughput screening on 746 most stable systems, and successfully identified *four* nonmagnetic topological materials (cf. Fig. 1).

In this project, we are going to design novel functional van der Waals materials, *i.e.*, heterostructures of 2D materials with different functionality to achieve mutual control of different order parameters. The work will be focused on but not limited to one/more of the following sub-directions:

1. high throughput design of novel 2D materials by massive prediction of stable 3D materials with layered structures;
2. investigation of 2D ferromagnetic materials, including the topological transport properties, tunability using external electric fields;
3. designing 2D ferroelectric materials with either in-plane or out-of-plane polarization, based on the modern theory of polarization;
4. stability and functionality of van der Waals heterostructures (cf. Fig. 2).

For the motivated candidates, expertise will be gained on parallel computation, coding with Python, and experience on DFT for his/her PhD study in the direction of theoretical materials science. Please write a message to Prof. Hongbin Zhang (email: hzhang@tmm.tu-darmstadt.de) or drop by in his office (L1|08, 404a).

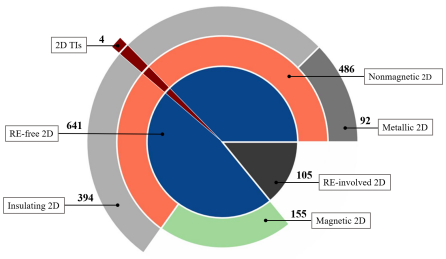

FIG. 1: Classification of 746 2D materials in the 2D materials database.

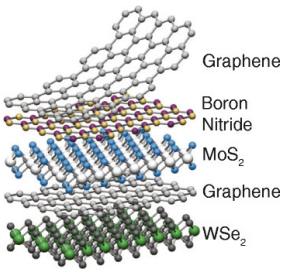

FIG. 2: Sketch of van der Waals heterostructures.