ARL/Master Thesis

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

TECHNISCHE UNIVERSITÄT DARMSTADT

High throughput Screening of Magnetic Ground States

Functional magnetic materials are critical for many emergent and cutting-edge technologies, such as magnetic cooling and spintronics. Recently, computational material design has been used to accelerate the discovery and guide the optimisation of magnetic materials. However, an open question is how to determine the magnetic ground state, such as ferromagnetic and antiferromagnetic, that determines the applicability and electronic properties of the material. A classical description for magnetism is found in the Heisenberg model, where the magnetic interactions are parameterised as exchange interactions (Jij). Such Jij's are reliably obtainable from ab initio codes such as SPR-KKR.

In this project, we are going to focus on establishing a methodology to determine the magnetic ground state from exchange interactions, accounting for how difference reference states (FM,AFM,PM) and what terms to include in the Hamiltonian (such as spin-orbit coupling), thus laying the ground work for a comprehensive description of the ground state within computational material design.

For the motivated candidates, expertise will be gained on parallel computation, coding with Python, and experience on sophisticated density functional theory calculations, valuable for both future PhD studies and industrial positions.

Please write Prof. Hongbin Zhang (Email: hongbin.zhang@tu-darmstadt.de) if you are interested.

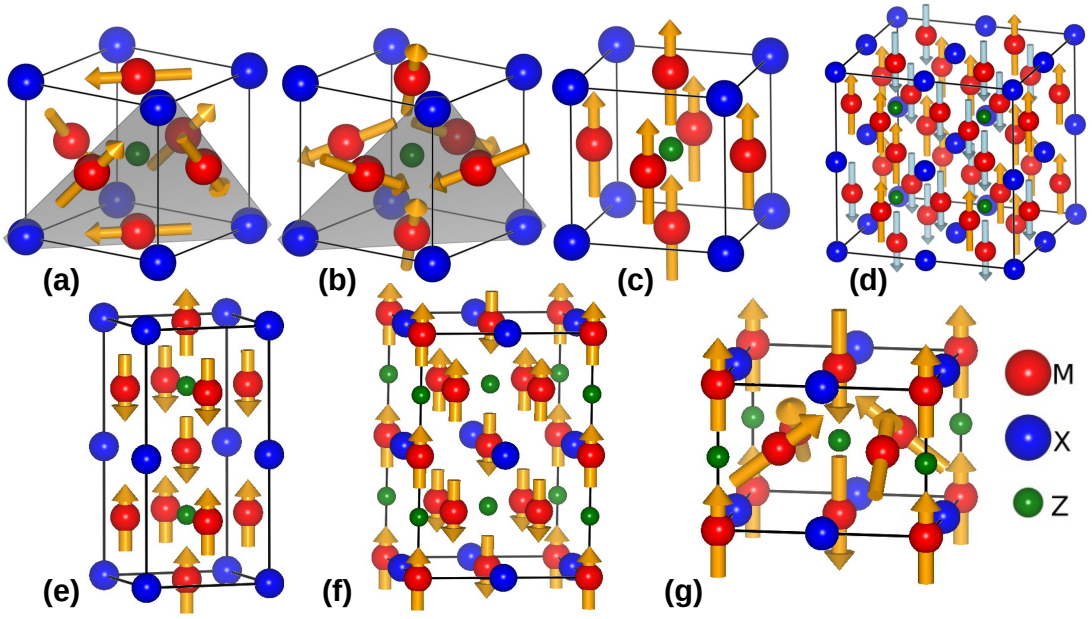

FIG. 1: Possible magnetic structures in antiperovskite compounds