CSC/DAAD PhD position

in the group of *Theory of magenetic materials*

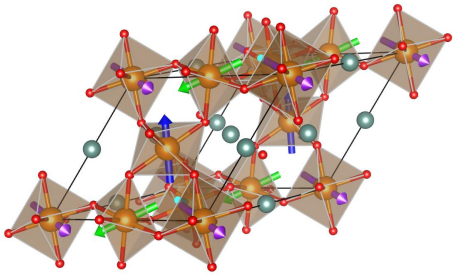
TECHNISCHE UNIVERSITÄT DARMSTADT

DFT+DMFT study of strongly correlated topological materials

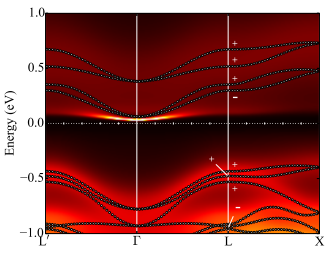
Topological phenomena, have been recently discovered in different nontrivial formulation in various materials, including topological insulators, Chern insulators, topological Weyl semimetals, and so on. Such studies have culminated in the Nobel Prize in physics 2016. Furthermore, it is well known that many emergent phenomena with peculiar properties (high-T_c superconductivity, multiferroics, *etc.*) can be induced by spontaneous symmetry breaking driven by Coulomb interaction between electrons in strongly correlated materials. The interplay of electronic correlations and the topological properties has not been well explored, *e.g.*, topological characterization of band gaps based on accurate electronic structure obtained using methods *beyond* density functional theory (DFT) with proper treatment of correlations is still missing for real materials.

The purpose of this project is to generalize the current implementation of the effective topological characterization based on state-of-the-art DFT and dynamical mean field theory (DMFT) methods, which has been applied successfully on pyrochlore iridates (arXiv:1505.01203, cf. figures below). We aim at extending and applying the current DFT+DMFT methodology for a consistent treatment of spin-orbit coupling and local electronic correlations to obtain accurate electronic structure, and then to evaluate various topological invariants following the simplified interacting topological theory. While a particular focus falls on the topological characterization of correlated insulating materials, as well as explicit exploration of the surface states therein by performing calculations in the slab geometry, we also dedicate special attention to semimetallic systems with nontrivial topological nature together with quantitative evaluation of benchmarking transport properties.

Candidates shall have a solid knowledge of solid state physics, experience with performing DFT calculations, and proficient English capabilities. Access to large-scale computational facilities and various codes are guaranteed in the group. The work will be carried out in collaboration with trend-leading groups in the US and Europa, with possibility of short-term visiting at different groups. We are fully supportive of applying for the CSC/DAAD scholarship. Please send your CV and a cover letter to Prof. Hongbin Zhang (email: hzhang@tmm.tu-darmstadt.de).



Primitive unit cell of pyrochlore iridates with all-in-all-out magnetic structure.



DFT+DMFT spectral function and the effective topological band structure of $Y_2Ir_2O_7$.