ARL/Master Thesis

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

TECHNISCHE UNIVERSITÄT DARMSTADT

High throughput Design of Fe_2P-type Magneto-caloric Materials

Magnetic cooling is a promising eco-friendly alternative to the conventional vapour-compression cycle, by exploiting the magneto-caloric effect (MCE). The MCE is greatly enhanced by a large entropy change concurrent with a discontinuous magnetisation change in a 1st order transition. Underlying this is a rich physical picture, involving magneto-structural coupling, metamagnetism and magneto-volume coupling effects. The Fe_2P-type family is known to host large MCE involving a first order transition.

In this project, we will set out to discover new compounds of such a structural type, along with doping mechanisms to optimize their MCE based on density functional theory calculations. The codes and workflows have been developed and tested on other materials systems in the group, where the stability, electronic structure and finite temperature magnetic properties will be evaluated.

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.

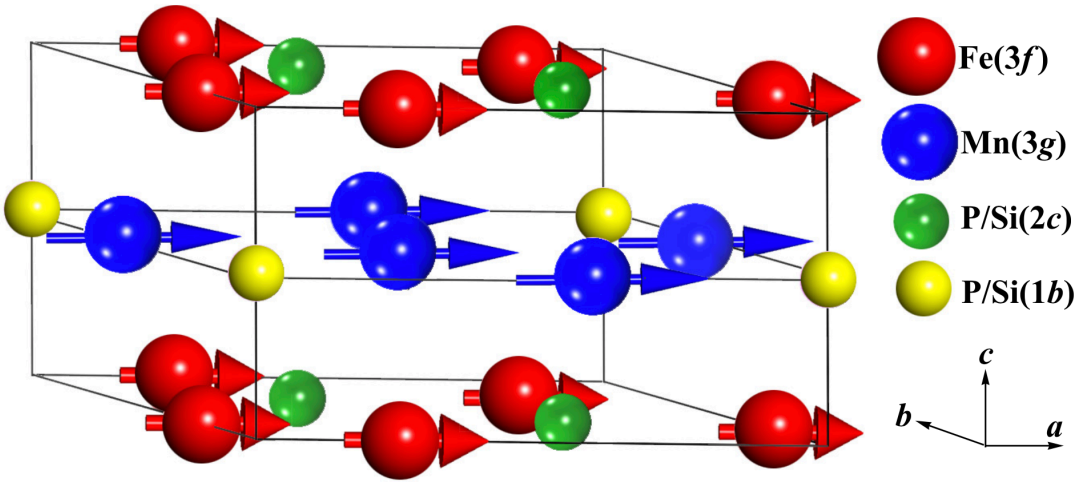

FIG. 1: Sketch of the Fe_2P-type crystal structure