



Designing permanent magnets by interstitial and substitutional doping

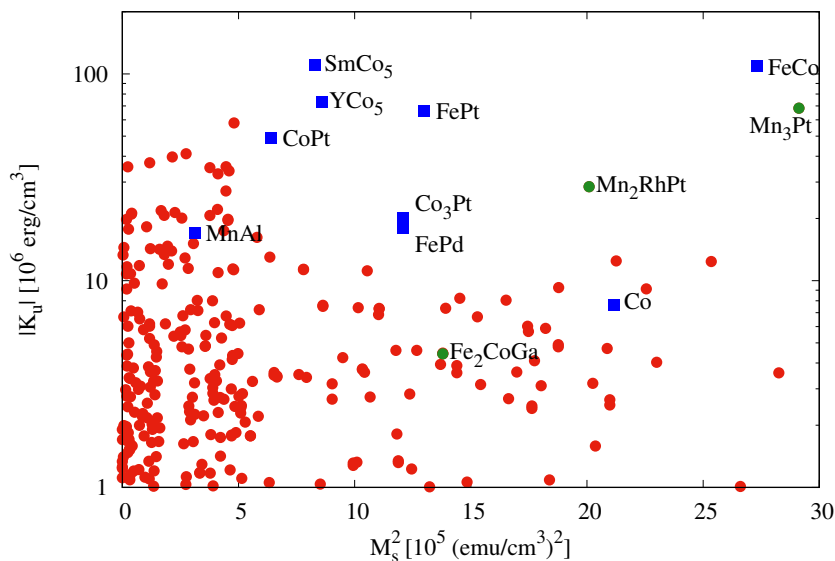
Based on our recent progresses of designing permanent magnets via tetragonalization induced by light interstitial (H, B, C, and N) atoms, we are looking for capable hands to continue in the line to optimize the magnetic properties by interstitial and substitutional doping. Assisted by high throughput calculations, the thermodynamic stability of a vast spectra of structural variations will be evaluated to identify the site occupation preference, followed by explicit evaluation of the magnetocrystalline anisotropy. The targeted material systems are

- compounds with $L1_0$ structure, such as FeNi, MnGa, FePt, CoPt, FePd, etc.
- Mn-based compounds, such as MnBi, Mn_3Ga , etc.

The expertise obtained by the prospective students are but not limited to:

1. proficiency in linux, python, and DFT (particularly spin-orbit coupling driven physics)
2. capability of performing high throughput calculations using supercomputers
3. hands-on experience with the in-depth characterization of intrinsic magnetic 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.



High throughput screening for permanent magnets via tetragonalization