Title : First-principles theory of high-performance permanent magnets

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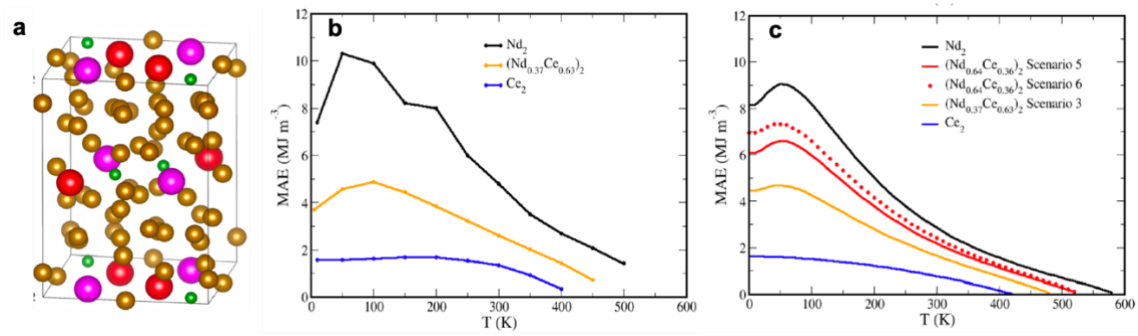
Research Area: Condensed Matter Physics, Material Science

Methods: first-principles electronic structure calculations (density-functional theory + dynamical mean-field theory); crystal-field theory; effective Hamiltonians

PhD track subject: High-performance permanent magnets are ubiquitous in modern industry playing a key role in sustainable power generation and transportation (e.g., in wind turbines and electric cars). Modern permanent magnets are complex multi-phase systems, which high performance is due to intermetallics of rare-earth and transition-metal elements. Transition metal elements, like Fe or Co, provide their high magnetization density, while rare-earth elements ensure a strong uniaxial anisotropy and magnetic hardness. The best existing permanent magnets are based on the $Nd_2Fe_{14}B$ intermetallic with heavy-rare-earth admixtures (Dy or Tb) further enhancing their performance at elevated temperatures. Volatile prices and scarcity of heavy rare-earth elements have recently become a serious issue. Significant research efforts are thus directed towards finding new high-performance permanent magnets with reduced rare-earth concentration.



a). Crystal structure of the $Nd_2Fe_{14}B$ permanent magnet. The purple and red balls are rare-earth atoms at two crystallographically different sites, the brown and small green balls are iron and boron, respectively. b) and c) show experimenta (b)l and calculated (c) magneto-crystalline anisotropy (intrinsic magnetic hardness) for various substitutions of Nd by the cheaper rare-earth element Ce. "Scenarios" refer to various models of Ce distribution over the rare-earth sites. Adapted from Ref. 4.

The goal of this project to develop an ab initio framework for predicting intrinsic magnetic properties of prospective rare-earth permanent magnets. This framework will simultaneously treat quasi-atomic 4f electronic shells of rare-earth with itinerant magnetism of the transition-metal sublattice. Ab initio calculations will determine key parameters for an effective model of magnetism in these compounds and provide input to larger-scale micromagnetic simulations or machine learning. The project will build upon the previous efforts of our group in this domain, see Refs. 1-4 and an example shown in the Figure above.

References

1. P. Delange, S. Biermann, T. Miyake, and L. Pourovskii, Phys. Rev. B **96**, 155132 (2017).
2. L. Pourovskii et al. Phys. Rev. B **101**, 214433 (2020).
3. A. Galler et al. npj Quantum Materials **6**, 2 (2021).
4. J. Boust et al., Phys. Rev. Materials **6**, 084410 (2022).