Search for substitutes of hard-magnetic materials containing less critical elements by computational high-throughput screening

Christian Elsässer
Fraunhofer Institute for Mechanics of Materials IWM, Freiburg; christian.elsaesser@iwm.fraunhofer.de

The discovery and design of new hard-magnetic intermetallic phases for high-performance permanent magnets are addressed by means of efficient and predictive computational high-throughput-screening approaches. The challenge is to identify substitutes for established hard-magnetic materials like $Nd_2Fe_{14}B$, which have outstanding functionalities but also constraining criticalities. To find promising candidates for new hard-magnetic phases, quantum-mechanical screening calculations based on density functional theory (DFT) are carried out to search for crystal structures and chemical compositions of intermetallic phases composed of transition-metal, rare-earth, and further substitutional or interstitial alloying elements, which have comparably good intrinsic ferromagnetic properties but contain less amounts of critical rare-earth elements than, e.g., the most prominent compound $Nd_2Fe_{14}B$.

References

N. Drebov, A. Martinez-Limia, L. Kunz, A. Gola, T. Shigematsu, T. Eckl, P. Gumbsch, and C. Elsässer, *New J. Phys.* **15**, 125023 (2013); W. Körner, G. Krugel, and C. Elsässer, *Sci. Rep.* **6**, 24686 (2016).