INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Room IC 02-722

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New permanent magnet phases from computational design

The increasing realisation of environmentally friendly technologies goes along with the need of new raw materials and magnetic materials often play a key role. The increasing use of 'green technologies' has raised the demand for high performance permanent magnets to replace today's commercial $Nd_2Fe_{14}B$ magnets by materials with smaller environmental footprints. In addition, new permanent magnets are sought after which can fill the gap between ferrites and high performance magnets.

Computational design based on ab initio methods has been proven to be an efficient and accurate tool to identify new phases with tailored properties. We have applied two different approaches. Optimization/modification of known phases has been used to identify e.g. new rare earth lean phases based on the 1:12 ($ThMn_{12}$) structure. These phases have significantly less rare earth then commercial $Nd_2Fe_{14}B$ but need phase stabilizing elements which can reduce the magnetic performance. Several promising phases could be identified. Here, $YFe_{11.5}Ti_{0.5}(N)$ and $Nd_{0.5}Y_{0.5}Fe_{11}Ti(N)$ will be discussed.

High-throughput methods were exclusively applied to identify so far unexplored rare earth free magnets. One study focusses on existing systems consisting of a 3d and a 5d element plus maximum one other element. The initial structures were taken from ICSD and after a number of calculation and filtering steps 5 candidate phases could be extracted which were previously not discussed as permanent magnets. [1] Identifying novel phases was the goal of a second study where we focussed on Fe-rich binary systems. Using evolutionary algorithms as implemented in USPEX several new candidate phases with magnetocrystalline anisotropy energies above 1MJ/m^3 and Curie temperatures well above room temperature could be identified. [2]

[1] arXiv:1910.00548 [2] S. Arapan et al., PRB 101, 014426 (2020)