Predicting novel hard magnetic material structures utilising machine learning models

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In this work we intend to develop methods to predict stable composition of hard magnetic materials with the main motivation being reduction in use of rare earth elements in said materials. To such end a series of machine learning models have been developed to test datasets, feature representations, architectures, training approaches and targets. The as prepared models are intended to reduce the exploration space of possible material compositions and to allow to then confirm or reject suitable candidates using more established and accurate methods such as DFT calculations or actual experimental synthesis. Some simple models such as Random Forest models can provide a good basis for predicting several commonly sought after properties of magnetic materials. The publicly available datasets allow training good model foundations with further refinement requiring additional data provided via e.g. DFT calculations. Other models, such as those utilising graph neural networks, were then also trained to predict features, such as Curie temperature, that are more time consuming to predict using standard techniques.

References:

[1] Bo Zhao and Hongbin Zhang, Physical Review B, 111, 224428, (2025)
[2] H. Moustafa, et al. arXiv:2506.23615, [physics.comp-ph]. (2025).

We acknowledge the financial support of the National Science Center Poland under the decision DEC-2021/41/B/ST5/02894 (OPUS 21)