

Searching for free rare earth and rare earth free permanent magnets using machine learning

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The goal of the project is to discover replacements for currently used permanent magnets. The best performance magnets in use today, such as neodymium and samarium magnets, typically contain a few to tens of percent of elements whose availability and extraction is severely limited. Those elements whose availability has fluctuated widely in the past and whose extraction may not meet future demand include, among others, heavy rare earth elements such as neodymium, praseodymium and samarium, which are components of commonly used permanent magnets. In addition, the rapid growth of industry sectors such as electric cars, robotics and wind energy is driving ever-increasing demand for top-quality permanent magnets, which are essential to the operation of most electric motors and wind turbines. Therefore, in order to meet the growing demand for permanent magnets while reducing the negative environmental impact associated with the mining of neodymium and samarium, it is necessary to discover new materials that do not contain these critical elements in their composition. While the title concept of rare earth free permanent magnets is already understood, the symmetrical concept of free rare-earth permanent magnets means materials based precisely on lanthanum and cerium, which are obtained in large quantities during extraction of the desired neodymium and samarium from rare-earth oxides, thus as a by-product prices of lanthanum and cerium are moderate.

The planned research includes a dominant computational part and an experimental stage to verify the predictions. In the computational part, using machine learning algorithms, a universal model will be developed based on the extensive database we will prepare, which then will be used to predict optimal permanent magnet compositions. The database will be created from quantum mechanical calculations, called first-principles calculations, in which materials will be modeled at the atomic level in terms of the spatial distribution of nuclei and electrons. Optimal compositions obtained by machine learning algorithms, after successful theoretical verification, will be synthesized and characterized in the laboratory. The computational part of the project will be performed at the Poznan Supercomputing and Networking Center (PSNC) and the Institute of Molecular Physics of the Polish Academy of Sciences in Poznan. The project members will work closely with foreign partners from the Department of Physics and Astronomy at Uppsala University in Sweden.

Research conducted under the project will translate into the development of the research field and scientific discipline at three levels. At the highest level, new permanent magnet compositions will be identified that can be used in industry or become the basis for research at the level of microstructure optimization and further composition modifications. At the middle level, the foundations of numerical methods - machine learning based on first-principles calculations - will be developed that can find universal application in the search for new materials with desired properties. At the lowest level, first-principles calculations, new issues related to the use of the fully relativistic fixed spin moment method and the modeling of alloys based on multiple supercells will be developed.