Ab-initio screening for hard-magnets

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Abstract

High-throughput computational materials design is currently exploited in many fields of materials science, such as photovoltaic, battery technologies, energy saving devices, thermoelectric materials and even more recently to search for new topological insulators. By combining advanced DFT electronic-structure methods with intelligent data mining, database construction, crystal prediction methods and exploiting the power of current supercomputer architectures; scientists generate, manage and analyse enormous data repositories for the discovery of novel materials. Following this idea we endeavour in the search for new superhardmagnets, for which we propose a simple and a robust descriptor in order to evaluate possible candidates. In this poster we present: i) Brief description of our research methodology (algorithm and computational search). ii) Benchmarking of our current implementations and principal drawbacks of our methodology. iii) Latest results and efforts in order to find new super-hardmagnets containing less rare-earth metals.