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The magnetic genome project

STEFANO SANVITO, School of Physics, AMBER and CRANN Institute, Trinity College Dublin

Magnetic materials underpin a vast and diverse range of modern technologies, going from data storage to energy production and use. However, the choice of magnets for mainstream applications is limited to a few dozens and the development of a new high-performance magnetic compound is a long and often unpredictable process. Here we describe a systematic pathway to the discovery of novel magnetic materials for multiple applications, which demonstrates an unprecedented throughput and speed up in the discovery process. We have constructed a massive electronic structures library for Heusler alloys containing 236,856 materials. We have then extracted those magnetic compounds with specific electronic properties, such as half-metallicity and large magnetization density, and finally established whether these can be fabricated at thermodynamical equilibrium. Based on our analysis we have identified 249 stable new intermetallic Heuslers, including 21 new magnets. Our work paves the way for large scale design of novel magnetic materials at unprecedented speed.