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The magnetic genome project

Stefano Sanvito
School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

Every technology is intimately related to a particular materials set. The steam engines that powered the industrial revolution in the eighteenth century were made of steel and, information and communication technologies are underpinned by silicon. Once a material is chosen for a given technology, it gets locked with it because of the investments associated with establishing large-scale production lines. This means that changing the materials set in an established technology is a rare event and must be considered as a revolution. High-throughput computational materials design is an emerging new concept in materials science with the potential of making real some of such revolutions. By combining advanced thermo-dynamic and electronic- structure methods with intelligent data mining and database construction, and exploiting the power of current supercomputer architectures, scientists generate, manage and analyse enormous data repositories for the discovery of novel materials. Here I will review such concept of high-throughput computational materials design by considering the specific case of designing new high-performance magnets.

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 248 stable new intermetallic Heuslers, including 20 new magnets. Our work paves the way for large scale design of novel magnetic materials at unprecedented speed.