HIGH-THROUGHPUT ELECTRONIC STRUCTURE THEORY: ARE ALL CALCULATIONS USEFUL?

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The development of novel materials is a strong enabler for any technology, and often technology and materials innovation cannot be separated. Unfortunately the process of finding new materials, optimal for a given application, is lengthy, often unpredictable and has a low throughput. Here I will describe a systematic pathway to the discovery of novel materials, which demonstrates an unprecedented throughput and discovery speed. The method can be applied to any materials class and any potential application. I will use the example of magnetism to introduce the main features of the method, and I will demonstrate the discovery of several new high-performance magnets. Furthermore I will highlight how such high-throughout schemes can be combined with machine-learning methods for data-mining to extract novel materials designing rules and for identifying new prototypes for further investigation.

Based on an extensive electronic structures library of Heusler alloys containing 236,115 prototypical compounds, we have filtered those alloys displaying magnetic order and established whether they can be fabricated at thermodynamical equilibrium1. Specifically, we have carried out a full stability analysis for intermetallic Heuslers made only of transition metals. Among the possible 36,540 prototypes, 248 are found thermodynamically stable but only 20 are magnetic. The magnetic ordering temperature, TC, has then been estimated by a regression calibrated on the experimental TC of about 60 known compounds. As a final validation we have attempted the synthesis of a few of the predicted compounds and produced two new magnets. One, Co2MnTi, displays a remarkably high TC in perfect agreement with the predictions, while the other, Mn2PtPd, is a complex antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at unprecedented speed.

REFERENCES

1 Stefano Sanvito, Corey Oses, Junkai Xue, Anurag, Tiwari, Mario Zic, Thomas Archer, Pelin Tozman, Munuswamy Venkatesan, J. Michael D. Coey and Stefano Curtarolo, *Accelerated discovery of new magnets in the Heusler alloy family,* Science Advances 3, e1602241 (2017).