Accelerating Materials Discovery with Data-Driven Atomistic Computational Tools

Chris Wolverton

[1]Dept. of Materials Science and Eng., Northwestern University, Evanston, IL (USA)

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. Both the materials discovery and materials development processes may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory (DFT). Here, we present an overview of recent work utilizing high-throughput computation and data mining approaches to accelerate materials discovery, specifically highlighting three new approaches: (i) We describe our high-throughput DFT database, the Open Quantum Materials Database (OQMD), which contains over 280,000 DFT calculations and is freely available for public use at http://oqmd.org. (ii) We show how computational crystal structure solution may be addressed via a new hybrid approach, the First-Principles Assisted Structure Solution (FPASS) approach, which combines experimental diffraction data, symmetry information, and first-principles-based evolutionary algorithmic optimization to automatically solve crystal structures. (iii) We also describe a newly-developed machine learning approach to construct a materials screening model based on an extensive set of thousands of DFT calculations. The resulting model, which has "learned" rules of chemistry from these many examples, can predict the stability of arbitrary compositions *without* requiring any *a priori* knowledge of crystal structure, at about six orders of magnitude lower computational expense than the original QM tools. We use this model to scan—in a matter of minutes—roughly 1.6 million candidate compositions for novel ternary compounds ($A_xB_yC_z$), and predict roughly 4,500 new stable materials.

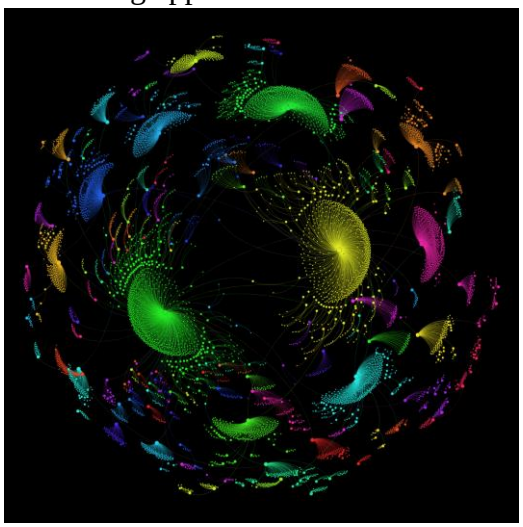

Fig. 1 A network graph containing (the minimum spanning tree of) all 7,410 DFT-predicted convex hull phases (points) from the Open Quantum Materials Database (OQMD) and their tielines to each other (lines).

References:

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Corresponding author*: c-wolverton@northwestern.edu