Using Machine-learning to Create Predictive Material Property Models and Accelerate Combinatorial Searches

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Abstract

Rational, data-driven materials discovery has the potential to make research and development efforts far faster and cheaper. In such a paradigm, computer models trained to find patterns in massive chemical datasets would rapidly scan compositions and systematically identify attractive candidates. Here, we present several examples of our work on developing machine learning (ML) methods capable of creating predictive models using a diverse range of materials data. As input training data, we demonstrate ML on both large computational datasets of DFT calculations, as implemented in the Open Quantum Materials Database (oqmd.org), and also experimental databases of materials properties. We construct ML models using a large and chemically diverse list of attributes, which we demonstrate can be used as an effective tool to automatically learn intuitive design rules, predict diverse properties of crystalline and amorphous materials, such as formation energy, specific volume, band gap energy, and glass-forming ability, and accelerate combinatorial searches.

Short Biography

Chris Wolverton is the Jerome B. Cohen Professor of Materials Science and Engineering at Northwestern University. Before joining the faculty, he worked at the Research and Innovation Center at Ford Motor Company, where he was group leader for the Hydrogen Storage and Nanoscale Modeling Group. He received his BS degree in Physics from the University of Texas at Austin, his PhD degree in Physics from the University of California at Berkeley, and performed postdoctoral work at the National Renewable Energy Laboratory (NREL). His research interests include computational studies of a variety of energy-efficient and environmentally friendly materials via first-principles atomistic calculations, high-throughput and machine learning tools to accelerate materials discovery, and "multiscale" methodologies for linking atomistic and microstructural scales. He has published over 250 papers with >17,000 citations and an h-index of 68. He is a fellow of the American Physical Society.