Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Novel energy materials through structural search MAXIMILIAN AMSLER, Northwestern University, STEFAN GOEDECKER, Basel University, CHRIS WOLVERTON, Northwestern University — Sophisticated structure prediction methods have been developed and become essential tools when designing new materials with desired properties. Their successful applications to many systems at various conditions and the increasing amount of available computational power have strongly contributed to their popularity.
The Minima Hopping Method (MHM) is a powerful tool to find low energy structures given only the chemical composition of a system and allows the prediction of structures at any boundary condition. Recently, not only the thermodynamic ground states, but also metastable phases accessible through various synthesis methods have drawn considerable interest for energy applications. We present the discovery of novel energy materials, ranging from low-density silicon allotropes with improved absorption in the visible to thermoelectric materials, by optimizing the MHM to imitate synthesis pathways.

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Date submitted: 05 Nov 2015 Electronic form version 1.4