Fall 2015 Joint Colloquium
Materials Department & Materials Research Laboratory

Professor Chris Wolverton
Dept. of Materials Science and Engineering
Northwestern University

Friday, November 20th, 2015
11:00 am, ESB 1001

Pizza served afterwards.

Materials Genome Approach to Computational Design of Nanostructured Thermoelectrics

Creating nanostructures within alloyed bulk thermoelectric materials can greatly decrease the lattice thermal conductivity of the material and thereby increase the thermoelectric efficiency of these materials. However, the rational design of thermoelectric alloys with even larger figures of merit will require a quantitative knowledge of the electronic and thermal properties and phase stability of nanostructured semiconductor materials. I will present key examples to show how first-principles based calculations can reveal the intricate but tractable relationships between properties for optimization of thermoelectric performance. The integrated optimization includes significant reduction of the lattice thermal conductivity with multi-scale hierarchical architecturing, large enhancement of Seebeck coefficients with intra-matrix electronic band convergence engineering, and control of the carrier mobility with band alignment between host and second phases. These techniques can simultaneously enhance the power factor and reduce the lattice thermal conductivity, thereby leading to high efficiency thermoelectric materials.

Bio Christopher Wolverton is a 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 and his PhD degree in Physics from the University of California at Berkeley. After completing his PhD degree, Wolverton 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 data mining tools to accelerate materials discovery, and "multiscale" methodologies for linking atomistic and microstructural scales. Wolverton has authored or co-authored ~200 peer-reviewed publications (h-index=52), holds nine patents (several others pending), and has given more than 150 invited talks. Wolverton is a Fellow of the American Physical Society, has won the Walder Award for Research Excellence, a Ford Motor Company Technical Achievement Award, and gave the John Dorn Memorial Lecture at Northwestern in 2003.

http://wolverton.northwestern.edu/

Hosted by Chris Van de Walle