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NEBRASKA CENTER FOR MATERIALS AND NANOSCIENCE SEMINAR SERIES PRESENTS

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DR. DEREK A. STEWART

Cornell Nanoscale Facility, Cornell University
Ithaca, New York

PREDICTING THERMAL TRANSPORT IN NANOSTRUCTURE AND MATERIALS FROM FIRST PRINCIPLES

While intensive research has focused on electrical transport for nearly a century, thermal transport has proven difficult to quantify and model. However, a predictive model for thermal conductivity can improve our understanding of nanoscale heat transport, thermoelectric materials, thermal resistance barriers, and even geologic heat transfer. In this talk, Dr. Stewart will discuss the development of a new first principles framework to model thermal transport in materials and nanostructures. Using density functional perturbation theory, we are able to calculate both harmonic and anharmonic interatomic force constants. Coupling these terms with a Boltzmann transport approach, we are able to demonstrate excellent agreement between the calculated and measured lattice thermal conductivities of technologically relevant semiconductors (silicon, germanium, and diamond) without the use of any adjustable parameters.

Nanoscale systems present unique opportunities for potential heat mitigation and thermoelectric applications. However, due to the atomic scale of these structures, their thermal transport properties can be significantly affected by impurities, defects, and even isotopic composition. In order to accurately model heat conduction in nanoscale systems, it is important to describe these systems using an approach that can model both interatomic interactions as well as structural relaxations due to defects. Dr. Stewart will discuss a non-equilibrium Green's function thermal transport approach that builds on interatomic force constants calculated from density functional theory. With this approach, we can reproduce the experimentally observed thermal enhancement in isotopically pure boron nitride nanotubes, examine potential nanoscale phonon localization effects, and also investigate the impact of Stone-Wales defects and symmetry breaking on thermal transport in carbon nanotubes. Finally, Dr. Stewart will discuss the exciting frontier of engineering phonons in nanostructures to develop new devices with specific thermal and electronic properties.

Derek Stewart received his B.S. in Physics (1996) from the University of Tennessee – Chattanooga, his M.S. in Engineering Physics (1998) at the University of Virginia (UVa), and his Ph.D. in Physics at UVa in 2001. During a postdoc at Sandia National Laboratories in Livermore, CA, Derek helped develop a first principles electronic transport code based on linear muffin tin orbitals and also examined photocurrents in nanotube p-n junction. Derek currently directs nanoscale simulation at the Cornell Nanoscale Facility and serves as the computational liaison for the National Nanotechnology Infrastructure Network. In addition to studying *ab-initio* thermal transport, he is also currently investigating the electronic properties of graphene oxide and the role of magnesium boron oxides in magnetic tunnel junctions.

Thursday
April 22, 2010
202 Brace
2:00 p.m.

Host:
Professor
Kirill Belashchenko
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