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Phonon Thermal Transport in Thermoelectric Materials from First Principles[1]

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Breakthroughs in nanoscience and materials fabrication technology have led to the creation of materials with very low lattice thermal conductivity [1, 2], a requirement for high thermoelectric efficiency. There is now an unprecedented need for quantitative, predictive theoretical approaches to provide fundamental understanding of lattice thermal transport in thermoelectric materials and insight into the design and development of new materials for enhanced thermoelectric applications. In this talk, I will describe our atomistic first principles approach for calculating lattice thermal conductivity of materials [3-6], which combines a complete solution of the Boltzmann transport equation for phonons with harmonic and anharmonic interatomic forces determined from density functional theory. I will present an overview of this theoretical approach along with some of our recent calculated results for a range of test materials such as Si, Ge and III-V compounds. I will also discuss results for thermoelectric alloys such as Si_xGe_{1-x} and $Mg_2Si_xSn_{1-x}$ and nanoparticle embedded in alloy thermoelectric (NEAT) materials. Finally, I will discuss insights gained from this effort such as the importance of anharmonic coupling of acoustic and optic phonon modes.

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[4] A. Kundu et al, Phys. Rev. B, 84, 125426 (2011);
[5] L. Lindsay et al., Phys. Rev. Lett. 109, 095901 (2012).
[6] W. Li et al, submitted (2012).

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