From Spins to Phonons: Applying Transport Lessons to First Principles Heat Transfer

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As a graduate student, I had the wonderful opportunity to work with Bill Butler at ORNL on giant magnetoresistance in magnetic multilayers and spin valves. This experience introduced me to a fascinating world of Green's functions, Boltzmann transport equations, coherent potential approximations, and the renowned trio of Korringa, Kohn, and Rostoker. Although I only worked with Bill for a few years, this foundation in transport theory has served me well throughout my career. In my talk, I will discuss my recent work on developing a first principles framework for thermal transport in materials and nanostructures. By incorporating *ab-initio* harmonic and anharmonic interatomic force constants into an iterative solution of the Boltzmann transport equation, we can predict phonon thermal conductivity in excellent agreement with experiment for numerous materials (e.g. Si, Ge, diamond)[1-3]. In addition, by linking these force constants to a ballistic Green's function approach, we can also examine how defects and impurities affect thermal transport in potential nanoscale heat conduits. I will highlight our recent studies on non-toxic thermoelectric alloys (e.g. SiGe, $Mg_2Si_xSn_{1-x}$) and discuss routes to modify the thermal conductivity via embedded nanoparticles[4], pressure, and size effects in nanowires[5,6]. I will also explore the impact of phonon localization on thermal transport in carbon and boron-nitride nanotubes[7,8]. Finally, I will discuss the impact of electronic transport concepts on our understanding of thermal transport and what lies ahead for the field.

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