First principles nanoscale phonon transport: insights and predictions

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The management of heat and the understanding of heat transfer are ubiquitous challenges in numerous sciences and technologies, from models of Earth's thermal history to managing local hot spots in microelectronics. Computational materials physics is now playing an increasingly important role in developing fundamental insights into the lattice thermal conductivity of solids, a fundamentally important parameter that determines the utility of a material for energy-related applications including thermoelectricity, nuclear power generation, heat dissipation and manipulation, and thermal analogs to electronic components (e.g., thermal diodes and switches).

Here I will discuss a powerful, predictive method for modeling heat transfer: first principles Peierls-Boltzmann transport. Discussion will focus on application of this method to examine lattice dynamics and transport in a variety of nanoscale systems (*e.g.*, wires, two-dimensional (2D) sheets and layered materials) – comparing with relevant experimental research. In particular I will present recent work related to strain, defects and chemical functionalization in 2D systems, and, if time allows, recent work applying Green's function methods for defect engineering.

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