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Predicting lattice thermal conductivity with help from *ab initio* methods[1]

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The lattice thermal conductivity is a fundamental transport parameter that determines the utility a material for specific thermal management applications. Materials with low thermal conductivity find applicability in thermoelectric cooling and energy harvesting. High thermal conductivity materials are urgently needed to help address the ever-growing heat dissipation problem in microelectronic devices. Predictive computational approaches can provide critical guidance in the search and development of new materials for such applications. *Ab initio* methods for calculating lattice thermal conductivity [1] have demonstrated predictive capability, but while they are becoming increasingly efficient [2], they are still computationally expensive particularly for complex crystals with large unit cells . In this talk, I will review our work on first principles phonon transport for which the intrinsic lattice thermal conductivity is limited only by phonon-phonon scattering arising from anharmonicity. I will examine use of the phase space for anharmonic phonon scattering and the Grüneisen parameters as measures of the thermal conductivities for a range of materials and compare these to the widely used guidelines stemming from the theory of Liebfried and Schölmann [3]. [1] D. A. Broido, M. Malorny, G. Birner, N. Mingo, and D. A. Stewart, Appl. Phys. Lett. 91, 231922 (2007); [2] Wu Li, J. Carrete, N. A. Katcho, and N. Mingo, Comp. Phys. Comm. 185, 1747 (2014); [3] G. Leibfried and E. Schlömann, Nach. Akad. Wiss. Gottingen,Math. Phyz. Klasse **4**, 71 (1954).

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