Ab-initio lattice thermal conductivity calculations for large libraries of compounds: Challenges and strategies

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Further development of technologies such as thermoelectric energy harvesting and power electronics demands compounds with lattice thermal conductivities optimized for each particular application. Given the high cost of experiment, predictive computational methods have a very important role to play in discovering new materials and in improving the efficiency of existing solutions. Due to advances in computing power, today it is feasible to solve the Boltzmann transport equation (BTE) for phonons using only data from *ab-initio* calculations, without any free parameters or experimental input. The first part of this presentation is devoted to discussing the main ingredients to such numerical approaches, which generally afford results in very good agreement with experiment for crystalline compounds. In a second part, our own implementation of the method [1] is presented. In combination with existing tools, our open-source software package SHENGBTE [2] enables researchers to build a workflow leading from an atomistic description of the crystal structure of a solid to the values of its lattice thermal conductivity and many related variables.

In spite of the success of numerical solutions to the BTE, many important challenges remain open. Some of those challenges are discussed in the final part of this presentation: the high computational cost of obtaining anharmonic interatomic force constants, the difficulty of evaluating convergence, the intrinsic limitations of DFT, the computational demands of complex unit cells and higher-order anhamonicity, and so forth. Those challenges become more relevant in the context of high-throughput explorations of large libraries of compounds, where the total number of CPU hours required can be very considerable. A number of strategies to overcome or mitigate them are listed.

[1] Wu Li, J. Carrete, N. A. Katcho, N. Mingo, Computer Physics Communications (in press).
[2] http://www.shengbte.org