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Thermal conductivity of bulk crystals from first-principles lattice dynamics[1] KEIVAN ESFARJANI, MIT, JUNICHIRO SHIOMI, University of Tokyo, GANG CHEN, MIT — Based on first-principles density-functional calculations, we have developed and tested a force field for Silicon, which can be used for Molecular dynamics simulations and the calculation of its thermal properties. This force field uses the exact Taylor expansion of the total energy about the equilibrium positions up to 4th order. In this sense, it becomes systematically exact for small enough displacements, and can reproduce the thermodynamic properties of Si with high fidelity. Having the harmonic force constants, one can easily calculate the phonon spectrum of this system. The cubic force constants, on the other hand, will allow us to compute phonon lifetimes and scattering rates. Results on equilibrium Green-Kubo molecular dynamics simulations of thermal conductivity as well as an alternative calculation of the latter based on the relaxation-time approximation will be reported. The accuracy and ease of computation of the lattice thermal conductivity using these methods will be compared. Results on other non-trivial materials such as Heuslers will also be presented. This approach paves the way for the construction of accurate bulk interatomic potentials and force constants database, from which lattice dynamics and thermal properties can be calculated and used in larger scale simulation methods such as Monte Carlo.

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