Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Lattice Thermal Conductivity of Silicon from DFTB Molecular Dynamics YINGHUI REN, Beijing Computational Science Research Center, TAO SUN, University of Chinese Academy of Sciences, DONG-BO ZHANG, Beijing Computational Science Research Center — Bulk and nano-structure silicons are promising building blocks for the design of future electronic devices. Understanding of their thermal conductivity is important not only for fundamental research, but also to develop applications, e.g., thermoelectricity. However, accurate measurement of thermal conductivity is challenging due to numerous experimental uncertainties. In this work, we develop a hybrid approach combining Born-Oppenheimer molecular dynamics (BOMD) with lattice dynamics. This approach depicts numerically phonon quasiparticles, from which the phonon lifetime $\tau(q,\lambda)$, group velocity $v(q,\lambda)$ and heat capacity $C_v(q,\lambda)$ are extracted for each phonon mode (q,λ). With these quantities, it is straightforward to evaluate the lattice thermal conductivity κ according to the Boltzmann transport equation, $\kappa = \frac{1}{3V}\sum_{q,\lambda} v^2(q,\lambda)\tau(q,\lambda)C_v(q,\lambda)$ To benchmark the validity of our approach, we carry out BOMD simulation and phonon calculation of bulk silicon using Density Functional based Tight Binding (DFTB) as implemented in the package of Trocadero. A series of temperatures from 300 to 1600 K are considered, and a good agreement with experimental data is achieved.

Yinghui Ren
Beijing Computational Science Research Center

Date submitted: 15 Nov 2016 Electronic form version 1.4