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Towards a First-Principles Method for Calculating Thermal Conductivity[1] ASEGUN HENRY[2], DAVID J. SINGH, ORNL — There are a number of areas where direct calculations of thermal conductivity based on first principles would be useful, particularly thermoelectrics. This could also be important in other areas, such as planetary science where thermal models for planet interiors often employ assumptions about properties of materials at extreme temperatures and pressures. Here we describe a framework for computing the instantaneous heat flux of a material in a first principles molecular dynamics method. The time history of the heat flux is then used to compute the thermal conductivity via the Green-Kubo formalism. Our formalism is different from that used in classical molecular dynamics because in first principles dynamics the energy is not uniquely decomposed into a sum of energies of individual atoms and the forces on an atom are not normally obtained as a sum of contributions from specific other atoms. The approach presented here has the benefit of generality, as it can be applied to any phase of matter in the limit that it is subjected to reasonable thermal gradients, where the system response is linear.

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