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A first-principles Green-Kubo method for thermal conductivity

JUN KANG, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory — Green-Kubo (G-K) method is widely used to calculate the thermal conductivity of materials. In this method, the thermal conductivity is related to the time correlation function of heat current. Up to date, the application of the G-K formalism is mostly limited in molecular dynamic (MD) calculations based on classic force-field. The combination of the G-K method with more accurate density functional theory (DFT) calculations is prevented by two issues: (i) the energy on each atom is needed to calculate the heat current and (ii) the heat current in the original G-K formalism is ill-defined for a periodic system. In this work, we address the two issues and develop a first-principles G-K method. We obtain an energy density based on the total energy formalism in DFT, and decompose it into each atom by using the charge density of the corresponding isolated atom as a weight function. For the calculation of heat current, we divide each MD step into two sub-steps, and create boundaries with zero heat current in each sub-step. The heat current within the boundaries is well defined and can be properly calculated. Finally we apply the proposed method to liquid argon. The results agree well with those obtained from classic MD calculations, indicating the validity of our method.

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