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An ab initio study of the effect of host-guest interaction on thermal transport in $Ba_8Ga_{16}Ge_{30}$ TERUMASA TADANO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo — Inorganic clathrate compounds are promising candidates for the next-generation thermoelectric devices because of their low lattice thermal-conductivities. In these materials, rattling vibrations of guest ions inside host cages are considered to play a significant role in reducing the lattice thermal-conductivity. In order to elucidate the microscopic mechanism of the reduction more clearly, we have performed first-principles analyses on a type-I clathrate $Ba_8Ga_{16}Ge_{30}$. Firstly, we calculated harmonic and anharmonic force constants of the material using the direct-method. Then, phonon scattering probabilities are evaluated from the imaginary part of the phonon self-energy. Our analysis shows that host-guest interactions increase the scattering probability of acoustic modes by one order of magnitude, and also cause a 10-fold reduction in the lattice thermal-conductivity. In addition, we observe that phonon mean-free-paths are far larger than the separation of Ba atoms, indicating that Ba atoms cannot be considered as individual scattering centers.

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