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First-principles calculation of lattice thermal conductivity of MgO JIANJUN DONG, BIN XU, Auburn University, CHRIS BROWN, Auburn University, JEFFREY NICKERSON, Auburn University — Lattice thermal conductivity of MgO has been calculated based on the first-principles total energy theory and the Boltzmann transport theory. In this study we consider the the anharmonic interaction up to the third-order. An efficient Brillouin zone integration technique is adopted to reduce the computational loads of calculating the phonon- phonon interaction terms in the linearlized Boltzmann equation. Our first-principle calculated results will be discussed with comparison to experimental data and some previous theoretical results.

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