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First-principles calculation of lattice anharmonicity and lattice thermal conductivity of MgSiO3 perovskite XIAOLI TANG, ABBY KAVNER, UCLA, JIANJUN DONG, Auburn University, UCLA COLLABORATION, AUBURN UNIVERSITY COLLABORATION — MgSiO3 perovskite (Mg-pv) is likely the most abundant material in the Earth's lower mantle, and its thermal conductivity at the high pressure and high temperature conditions of the Earth's interior plays an important role in governing heat transport and thus the whole Earth evolution. Measurement of the lattice thermal conductivity (κ) of this important material is still not available at lower mantle conditions. We will present a theoretical study of κ for Mg-pv calculated with a parameter-free method which combines first-principle techniques, quantum scattering theory, and kinetic transport equation. We have explicitly calculated the pressure dependence of both harmonic phonon spectra and the third order lattice anharmonicity tensors. A preliminary analysis based on the single relaxation time approximation suggests that the increase of phonon frequencies at high pressures contributes to the increase of κ at the rate of $1\% GPa^{-1}$ at 1000K and $1.3\% GPa^{-1}$ at 3000K. The pressure dependence of phonon relaxation time and its implication for the pressure dependence of κ will also be discussed.

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