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First-principles calculation of thermal conductivity of silicate perovskite at high pressures and high temperatures[1] JIANJUN DONG, Auburn University, XIAOLI TANG, California Institute of Technology, ABBY KAVNER, UCLA, MOSES NTAM, Auburn University — The lattice thermal conductivity of silicate perovskite, the most abundant mineral in the Earth's lower mantle, is calculated by combining the first-principles electronic structure theory and Peierls-Boltzmann transport theory. The phonon scattering rate due to lattice anharmonicity and Mg/Fe mass disorder is evaluated for each mode at the extreme P-T conditions of the lower mantle. The predicted thermal conductivity of single crystal MgSiO3 perovskite at ambient condition, about 5.7 W/m/K, is in excellent agreement with experiment. Adding about 6% Fe will lower the thermal conductivity by nearly 40%. Our calculation also reveals an unique pressure dependence for the thermal conductivity of perovskite, and the calculated thermal conductivity of iron bearing perovskite is almost an order of magnitude lower than the previously estimates based on long extrapolation of single crystal data. Including a re-evaluation of radiative contribution, we discuss the implications of our results for the heat flow in deep Earth.

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