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Thermal Conductivity of the Lowermost Mantle

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Thermal conductivity (k) of candidate deep-Earth mineral phases at high pressure and temperature represent a key parameter to understanding the thermal state of the deep Earth, and place important boundary constraints on convection in the outer core by which the magnetic field is generated. Current estimates for k in the lower mantle are very poorly constrained, ranging between $4 - 16\,\mathrm{W/m\,K}$. The large uncertainty results mainly from two factors. Firstly, measurements of k at pressure are extremely challenging and often mutually inconsistent, resulting in notable uncertainties. Secondly, there is no consensus on how to represent the pressure dependence of k; different models yield very different extrapolations. Due to the large uncertainties and a relatively small range in pressure in the experimental data, distinguishing among these various models was not previously possible.

We apply a simple and computationally efficient method for computing lattice thermal conductivity which combines equilibrium First-Principles Molecular Dynamics and Lattice Dynamics to compute the lattice conductivity of MgO periclase for a range of densities that span pressure values from ambient conditions to those characteristic of deep planetary interiors ($\sim 150\,\mathrm{GPa}$). Combining high pressure results with associated thermodynamic properties illustrates that Debye theory gives an excellent description of the pressure dependence of thermal conductivity in oxides. Results further reveal that acoustic modes are longer lived than optic modes by more than a factor of two. Combined with the notably higher group velocities of acoustic phonons, this suggests that Debye theory should also hold in more complex compounds with more optic modes. First-principles results for MgO periclase are subsequently combined with a Debye theory extrapolation of experimental estimates of thermal conductivity in $\mathrm{MgSiO_3}$ perovskite, to estimate the thermal conductivity at the base of the Earth's lower mantle.