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Thermal property modeling of the core-mantle boundary

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Lattice thermal conductivity of minerals under pressure and temperature is a key property to understanding dynamics and evolution of the Earth's interior. We recently established an efficient ab initio technique for calculating the thermal conductivity of silicate minerals with complex structure and chemistry (Dekura, Tsuchiya, Tsuchiya, PRL, 2013). Calculated lattice thermal conductivity of MgSiO3 perovskite agreed satisfactorily with experimental values at room temperature, and post-perovskite was found to have thermal conductivity quite different from perovskite's, indicating that the D" discontinuity is not only the phase transition boundary but also the conductivity boundary. Using the obtained results, we determine the effective conductivity of the lower mantle and estimate the energy flow across the core-mantle boundary (CMB). Our results demonstrate that the CMB heat flux could change significantly from place to place by reflecting temperature heterogeneity located atop the core. A large CMB heat flow recently suggested from the outer core side can be reconciled only by considering polycrystalline assemblages yielding high-thermal conductivity.

Keywords: First principles computation, Thermal conductivity, CMB heat flow