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Atomic-Scale Investigation of Thermal Conductivity in Lower Mantle Minerals

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Understanding heat transport across the core-mantle boundary (CMB) is essential for constraining Earth's thermal evolution and the dynamics of its magnetic field. Here we quantify the lattice thermal conductivity of key lower-mantle minerals: periclase, bridgmanite, and post-perovskite, under geophysically relevant pressure-temperature-composition (P-T-X) conditions. Our methodology combines the Boltzmann Transport Equation (BTE), Green-Kubo Molecular Dynamics (GKMD), and Non-equilibrium molecular dynamics (NEMD) within a unified, cross-validated framework that remains robust up to 150 GPa and 4000 K. To extend both accuracy and accessible length and time scales, we incorporate machine-learning interatomic potentials (MLIPs) based on advanced architectures such as MACE, enabling ab initio-quality predictions of phonon-mediated heat transport across strongly anharmonic regimes. We further explore compositional effects in Fe-bearing periclase and observe a pronounced reduction in thermal conductivity for $Mg_{0.75}Fe_{0.25}O$ compare to MgO, highlighting the importance of disorder scattering for deep-mantle heat transport. This ML-accelerated, multi-method approach provides improved constraints on mineral-scale conductivity relevant to CMB heat flux and Earth's long-term thermal evolution.