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Ab initio lattice thermal conductivity of deep mantle minerals

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The core-mantle boundary heat flow depends on the thermal conductivity of the base of Earth's lower mantle. Direct measurement of thermal conductivity of minerals remains technically challenging at the deep mantle condition. On the other hands, *ab initio* computational technique based on the density functional theory (DFT) allows us to examine microscopic process of the transport phenomena including the lattice thermal conduction. Earlier theoretical works calculated the lattice thermal conductivity of MgO with *ab initio* molecular dynamics (MD) simulation or direct evaluation of third-order anharmonic force constants to compute phonon-phonon interaction (Nico de Koker, Phys. Rev. Lett. **103**, 125902, 2009, X. Tang and J. Dong, Proc. Natl. Acad. Sci. U.S.A. **107**, 4539, 2010). However, in these approaches, the simulation cell is often insufficient to accurately calculate the long wave-length phonon-phonon interactions. This leads to a lack of the decay channels for the phonons. For a more reliable way, the anharmonic coupling between phonon modes can be calculated within density functional perturbation theory (DFPT). In this approach, the higher-order force constants are calculated based on the perturbative scheme taking care only of the primitive cell. In this presentation, we show the phonon decay and the lattice thermal conductivity of MgO in the lower mantle conditions.

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Keywords: first principles calculation, lattice thermal conductivity, phonon-phonon interaction, deep mantle minerals