Ab initio anharmonic lattice dynamics calculation for Fe-bearing lower mantle minerals

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Determination of lattice thermal conductivity (κ_{lat}) of lower mantle minerals is key to understanding the dynamics of the Earth' s interior. Although it was impractical in the deep Earth pressure (*P*) and temperature (*T*) condition for a long time, recent experimental and computational developments have been extending the accessible *P* and *T* ranges. We recently succeeded in developing an *ab initio* technique to calculate κ_{lat} at any *P* and *T* condition based on the density-functional theory (DFT) combined with anharmonic lattice dynamics theory. The technique was then applied to major end-members of lower mantle minerals, $MgSiO_3$ bridgmanite (Dekura,Tsuchiya,Tsuchiya,2013,PRL) and MgO periclase (Dekura,Tsuchiya,2017,under review). Next we extend our technique to more realistic Fe-bearing minerals in conjunction with the internally consistent LSDA+*U* technique (Wang,Tsuchiya,Hase,2015,Nature geoscience) to deal with such strongly-correlated systems. In this presentation, we introduce the current situation of our research on κ_{lat} .

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