学术报告(11.16 周三)

题 目: Lattice thermal conductivity of materials under high pressure and temperature from first principles

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摘要

Determination of lattice thermal conductivity (k) of Earth's lower mantle minerals is a key to understanding the dynamics of the Earth's interior. Although determination of k was impractical in the deep Earth P, T condition for a long time, recent experimental and computational developments have been extending the accessible P and T ranges. *Ab initio* prediction of k requires understanding of the phonon-phonon interaction associated with the lattice anharmonicity. I recently succeeded in developing an efficient method to calculate it based on the density-functional theory combined with knowledge on many body anharmonic phonon physics. Next, I extend the techniques to lower mantle minerals such as MgO and $MgSiO_3$, and now calculations of more realistic Fe-bearing systems are also started. In this presentation, I introduce the current situation of my research on k.

报告人简介

Haruhiko Dekura received his PhD in theoretical condensed matter physics from Osaka University in 2010 and then worked as a postdoctoral researcher in the Ecole Polytechnique of France and the Senior Research Fellow Center of Ehime University of Japan. From 2013, he started as an assistant professor in the Geodynamics Research Center of Ehime University mainly focusing on the simulations of material and mineral properties under the high pressure and high temperature conditions including thermal conductivity, phase transition, and superconductivity.