The 385th Geodynamics Seminar

Development in *ab initio* thermal transport property using the quantum perturbation theory applied to geophysics

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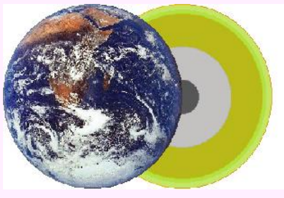

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Thermal transport properties such as thermal conductivity and viscosity are keys to understanding dynamics and therefore evolution of the Earth's interior. Despite the importance, the direct determinations of those physical quantities have long been unconstrained at high-pressure and -temperature, primarily owing to experimental difficulty. We recently developed an efficient *ab initio* computational method for lattice thermal conductivity of silicate minerals with complex structure based on the quantum perturbation theory, and applied it to $MgSiO_3$ perovskite (Dekura, Tsuchiya, Tsuchiya, PRL, 2013). The technique was next applied to $MgSiO_3$ post-perovskite (Mg-PPv) controlling dynamics of Earth's deep mantle. Meanwhile, to take into account the phonon-impurity scattering and its effect on the lattice thermal conductivity, we have been developing a new method ('*real-space method*') to extract anharmonic force constants from the higher order derivatives of the adiabatic potential surface. In this presentation, I will talk about each of these topics, and also discuss future perspectives.

詳細は当センターホームページ：http://www.ehime-u.ac.jp/~grc/をご覧ください
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