# Thermal and Chemical Interactions between the Core and Mantle

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The core-mantle boundary (CMB), where the silicate mantle directly contacts the iron core, is the largest boundary in the Earth. The core and mantle interact with each other physically and chemically at the CMB, and those interactions might control the evolution of the Earth's interior. For example, elemental partitioning between iron and silicate during the core formation process and also at the present CMB might affect the chemical evolution of the outer core. Also, the cooling rate of the core and thus the geodynamo activity significantly depend on the heat flow from the core to mantle. However, related physical and chmecal properties such as partitioning coefficients and thermal conductivity at high-P,T remain largely unclear.

We have therefore started developong theoretical techniques to investigate those properties based on the ab initio density functional framework, (1) the direct anharmonic lattice dynamics (ALD) method + Boltzmann transport equation (BTE) for lattice theraml conductivity (Dekura and Tsuchiya, 2017,2019,in prep.) and (2) the one-step thermodynamic integration (TI) + ab initio molecular dynamics (AIMD) method for liquid free energy then metal-silicate partitioning coefficient (Taniuchi and Tsuchiya, 2018; Xiong et al., 2018; Xiong and Tsuchiya, under review).

Calculated thermal conductivities of the major lower mantle phases (ferropericlase, bridgmanite, and post-perovskite) suggest the CMB heat flow less than 10 TW, which is distinctly smaller compared to the conductive heat flow proposed for the outer core expected from its considerably larger thermal conductivity (de Koker et al., 2014; Pozzo et al., 2014; Ohta et al., 2016). On the other hand, calculated liquid iron-silicate melt partitioning properties suggest that noble gases and water (hydrogen) both remain lithophile at 135 GPa but the core could have stored enough amount of promordial helium. Geophyscal insights drawn from these new results will be discussed in the presentation.

Keywords: Ab initio density functional calculations, Thermal conductivity, Metal-silicate elemental partitioning

 