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2024.06.21 (Fri.) 16:30 ~

Venue: Meeting Room #486
Science Research Bldg. 1, 4th floor.
Ehime Univ.

Keywords:
1. Carbon partitioning
2. Core-mantle differentiation
3. Thermodynamic integration

Carbon partitioning during core-mantle differentiation constrained from ab initio simulations

Carbon, as an Earth's major volatile element, plays a key role in regulating the climate and habitable surface environment, and is extensively involved in mantle dynamical processes. The abundance of carbon in the bulk silicate Earth (BSE) is estimated to be 90~130 ppm. And the BSE is characterized as super-chondritic C/N, sub-chondritic C/H and chondritic C/S ratios. Understanding the origin of such features is essential to unveil the origin and delivery of life-essential volatile elements and requires the knowledge of their partitioning behaviors during core-mantle differentiation.

Among these elements, the results of carbon partition coefficients under high-pressure and high-temperature are highly controversial. For instance, previous experiments conducted at relatively low pressures (< 8 GPa) have shown that carbon is strongly siderophile and becomes more with increasing pressure. In contrast, experimental and theoretical evidences demonstrate that carbon is much less siderophile at pressures of 35~60 GPa, though those data scatter more than an order of magnitude.

In this seminar, I will present the data of carbon partition coefficients between liquid iron and molten silicate acquired by *ab initio* molecular dynamics simulations combined with the thermodynamic integration technique. We find that the partitioning behavior of carbon varies under different chemical conditions, which is likely attributed to the change of the bonding environment of carbon in the silicate melt. These results help to reconcile the large discrepancies among experimental results. Furthermore, combining geochemical observations and modelling, I will discuss the distribution of carbon in the deep Earth.