THE GEODYNAMICS SEMINAR

№644

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Geodynamics Research Center

2025.11.28 (Fri.) 16:30 ~

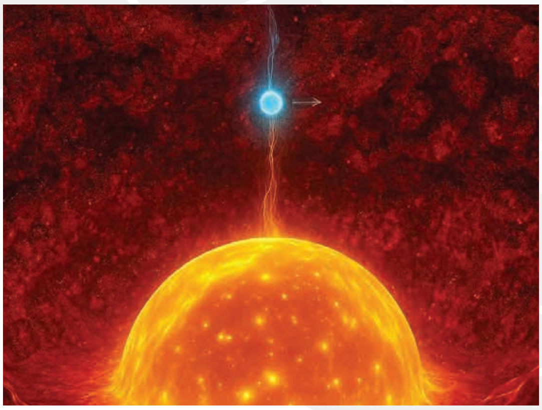
Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.

Ehime Univ.

Keywords

1. Core mantle differentiation
2. Sulfur Partitioning
3. Ab initio calculation



First-principles study on sulfur partitioning between metal and silicate at high pressure and temperature: Evolution of sulfur concentration in the deep Earth during the proto-Earth growth

S is one of the promising light elements that can explain the density deficit of the core (Birch, 1952). The degree of siderophile nature of S under high pressure and temperature (P,T) is key to estimating the S content in the core. However, a significant discrepancy between metal-silicate partition coefficient of S extrapolated from relatively low-pressures and measured at deep mantle P,T is identified (Rose-Weston et al., 2009; Suer et al., 2017). In this study, we investigated the partitioning behavior of S between liquid iron and molten silicate using first-principles free energy simulations based on the density functional theory (Hohenberg and Kohn, 1964; Kohn and Sham, 1965) and the thermodynamic integration method (Taniuchi and Tsuchiya, 2018), where the liquid state is reproduced using the molecular dynamics method. The results indicate that S is strongly siderophile at 0-135 GPa and 3000-5000 K, the partition coefficient markedly decreases with increasing the O in liquid iron, but the effect of Si in liquid iron diminishes as pressure increases and becomes negligible at 60 GPa. The pressure dependence of the calculated partition coefficient for S is found to change around 20 GPa. These properties might reconcile the experimental conflicts and are interpreted based on the local structure of the liquids. The present S-depleted Earth's mantle is suggested to form by accreting primordial bodies with an oxygen content of 0-10 mol% in their cores. On the other hand, the core is likely to have a substantial amount of S for all the parameter conditions examined.

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