Dr. Taku Tsuchiya
Professor & Director
Geodynamics Research Center

2024.12.20 (Fri.) 16:30 ~

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

Keywords:
1. Iron charge disproportionation reaction
2. Ab initio thermodynamic integration molecular dynamics
3. Core formation in the proto-Earth

Ab initio calculations of the iron charge disproportionation reaction in silicate melts

It is widely thought that the accretion of materials during the growth of the proto-Earth caused a large-scale melting, resulting in the formation of magma oceans (MOs). Recently, high-pressure experiments have continuously reported that the charge disproportionation (CD) reaction of iron facilitates in molten silicates under high pressure as suggested in solids [Armstrong et al., 2019; Kuwahara et al., 2023; Zhang et al., 2024]. This implies that the iron CD reaction might lead to the nucleation of metal droplets in the MO, which might have had some contribution to the formation of a metallic proto-core through their gravitational separation from silicate melt. A considerable discrepancy is however seen in the pressure dependence of the iron CD reaction reported in these experimental outputs. And although theoretical approaches are worthy as well, no studies have been conducted on this reaction so far.

In this study, the thermodynamic stability and pressure dependence of the iron CD reaction in MO are directly evaluated from the Gibbs free energies of molten silicates containing divalent and trivalent iron ions and liquid iron calculated by a non-empirical first principles way. These are performed using the originally developed thermodynamic integration molecular dynamics program [Taniuchi and Tsuchiya, 2018] over a wide pressure range under different temperature and iron concentration conditions. In this talk, I will present the obtained pressure, temperature, and composition effects on the iron CD reaction and try to rationalize them from the microscopic point of view.