[EE] Evening Poster | S (Solid Earth Sciences) | S-IT Science of the Earth's Interior & Tectonophysics

[S-IT22]Interaction and Coevolution of the Core and Mantle in the Earth and Planets

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Recent observational and experimental investigations have significantly advanced our understanding of the structure and constituent materials of the deep Earth. Yet, even fundamental properties intimately linked with formation and evolution of the planet, such as details of the chemical heterogeneity in the mantle and light elements dissolved in the core, remained unclear. Seismological evidence has suggested a vigorous convection in the lower mantle, whereas geochemistry has suggested the presence of stable regions there that hold ancient chemical signatures. The amounts of radioactive isotopes that act as heat sources and drive dynamic behaviors of the deep Earth are also still largely unknown. We provide an opportunity to exchange the achievements and ideas, and encourage persons who try to elucidate these unsolved issues of the core-mantle evolution using various methods, including high-pressure and high-temperature experiments, high-precision geochemical and paleomagnetic analyses, high-resolution geophysical observations, geo-neutrino observations, and large-scale numerical simulations. Since this session is co-sponsored by geomagnetism, paleomagnetism and rock magnetism division of the SGEPSS, contributions in geomagnetism and geodynamo simulation are also encouraged.

[SIT22-P18]First-principles study on the site occupancy of Fe^{3+} in ferropericlase (Mg,Fe)O

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Keywords:Fe3+, ferropericlase, First-principles calculation

A high vacancy concentration due to the extrinsic mechanism is considered to be reproduced rheological property of Earth’s lower mantle via diffusion creep (e.g., Ita and Cohen 1998). Charge unneutral Fe^{3+} is one of the major impurities to create vacancies as the following reaction $3Mg^{×} → 2Fe^{\cdot} + V^{''}$. It has been experimentally reported that the site occupancy of Fe^{3+} changes from the octahedral site to the tetrahedral in MgO with increasing pressure around 15 GPa (Otsuka et al., 2010), leading to a further increase of the vacancy concentration in the octahedral site. However, little is known about the effects of Fe^{3+}/vacancy configuration and the spin transition on its site preference, the differences in chemical bonds around octahedral and tetrahedral Fe^{3+}. In this study, we investigate Fe^{3+} bearing MgO by using first-principles calculation methods based on the density functional theory up to 150 GPa. The tetrahedral occupation of Fe^{3+} is so fur not found in all the defect configurations and pressure condition examined, being not consistent with experimental findings.