## Geodynamics Seminar

## 第353回ジオダイナミクスセミナー

First principles investigations of hydrous phases under pressure: Implications for the transportation of water into the Earth's deep interior

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日時:4/12(金)午後4時30分~場所:総合研究棟I4F会議室





## Abstract

The global circulation of water in the earth is important to investigate the evolution history and dynamics of the earth, since the physical properties (e.g. atomic diffusivity, melting temperature, electrical conductivity and seismic velocities) of the constituent minerals are considerably changed by the presence of water. It is widely accepted that hydrogen is carried into the deep earth's interior by a suite of hydrous minerals such as the dense hydrous magnesium silicates (DHMSs) in the descending cold plate. However, high pressure behavior of DHMSs, especially the stability of phase D (MgSi2O6H2) which is the highest pressure phase of DHMSs has not been clarified so far. In this study, I explored the possibility of further phase transition and dissociation of phase D into the hydrous or anhydrous minerals by using first principles calculation. As a result, the high pressure phase transition of phase D to the new high pressure hydrous phase MgSiO4H2 plus stishovite occurs at about 40 GPa. This new hydrous phase is stable up to about 52 GPa and then dissociate into MgSiO3 perovskite and H2O (ice VIII) at static 0 K condition. Therefore, there is a possibility that this new phase in subducting slab takes over water and carries into the deeper part of earth's lower mantle. This new hydrous phase further extends the stability field of dense hydrous magnesium silicates and also opens the pathway toward the existence of high pressure phase of ice in the lower mantle conditions. The detail of the structure, elasticity, and the high pressure-temperature phase boundary determined by quasi-harmonic approximation will be shown and the possible geophysical implications will also be discussed at the presentation.