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First principles prediction of a new dense hydrous magnesium silicate

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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 has been reported that water is carried into the deep Earth's interior by 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 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. As a result, the new phase which has lower enthalpy than phase D has been found above about 40 GPa. 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. The detail of the structure 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.

Keywords: DHMS, first principles calculation, hydrous mineral, high pressure