First principles investigation of high pressure phase of AlOOH and FeOOH

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Knowing the mechanism of global water circulation and determination of total budget of water in earth's interior is very important for investigating the evolutional history of our planet. It has been believed that water is carried into the deep Earth's interior by hydrous minerals such as the dense hydrous magnesium silicates (DHMSs) which are also known as alphabet phases (phase A, superhydrous phase B, and phase D etc.) in the descending cold plate.

Recently, we have theoretically predicted the high pressure phase of phase D and experimentally confirmed the existence of this new DHMS in lower mantle pressure conditions (Tsuchiya 2013, Nishi et al. 2014). This phase has MgSiO4H2 chemical composition and named as phase H. At the lower mantle pressure conditions, Al and H-bearing SiO2, d-AlOOH, e-FeOOH and phase H may be the candidate of the relevant hydrous phases in the subducting slabs. Interestingly, the crystal structure of these hydrous phases are almost same and similar to the CaCl2 type structure. This suggests that these hydrous phases may potentially be able to make the wide range of solid solution. Some experimental studies already reported that Al preferentially partitioned into phase H and the stability of phase H drastically increased by incorporation of Al (Nishi et al. 2014, Ohira et al. 2014). In this study, we report the high pressure behaviors and the possibility of further phase transition of AlOOH and FeOOH using first principles calculation techniques in order to investigate the effect of Al and Fe on the stability of phase H.