First principles investigation of high pressure behavior of FeOOH

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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) in the descending cold plate. A numbers of researches have been conducted so far about the high pressure behaviors of DHMSs. In recent years, we found new DHMS, phase H, at lower mantle pressure condition and the solid solution between phase H and d-AlOOH has been proposed as the most important carrier of water in the deepest part of Earth’s mantle (Tsuchiya 2013, Nishi et al. 2014, Ohira et al. 2014). However, those hydrous minerals are actually not denser than surrounding (dry) mantle minerals (Tsuchiya and Mookherjee 2015) and the gravitational stability in deeper part of the Earth is questionable. Therefore, the effects of denser element such as Fe on the stability of DHMS are intimately connected to the ability of transportation of water into Earth’s deep interiors. In order to assess the effect of Fe on the phase relation of phase H and d-AlOOH, we first investigated the high pressure behavior of the end-member composition of this system, the e-FeOOH. We have found the new high pressure transformation of FeOOH in the lower mantle conditions both theoretically and experimentally. Here, I show high pressure structures and the physical properties of FeOOH polymorphs using first principles calculation and discuss the possible geophysical implications of these phases.