First principles determination of the stability field of the phase H (MgSiO$_4$H$_2$) at lower mantle conditions

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It is believed that water is carried into the Earth’s deep interior by hydrous minerals such as dense hydrous magnesium silicates (DHMSs) in the descending cold plate. A number of studies have been conducted to determine the high-pressure behaviors of DHMSs. In recent years, we discovered a new DHMS, phase H, stable at lower mantle pressure condition above ~ 40 GPa and the solid solution formed by phase H and d-AlOOH has been proposed as the most important carrier of water to the deepest part of Earth’s mantle (Tsuchiya 2013, Nishi et al. 2014, Ohira et al. 2014, Panero and Caracas 2017).

However, the MgSiO$_4$H$_2$ phase H has been reported to decompose into H$_2$O (ice VIII) and MgSiO$_3$ perovskite at relatively low pressure condition about 52 GPa at 0 K by first principles calculation (Tsuchiya 2013). High temperature dissociation phase boundary between phase H and MgSiO$_3$+H$_2$O has not been determined so far, since the hydrogen disordered ice VII phase is stabilized above ~100 K around 50 GPa. Here we report the dissociation phase boundary of phase H at high pressure and temperature condition by determining the free energies of H$_2$O ice-VII (Umemoto et al. 2010) and MgSiO$_3$ perovskite (Tsuchiya et al. 2004) and discuss the possible scenario of the transportation of water into deep Earth interiors.