First principles determination of the stability field of the phase H ($MgSiO_4H_2$) 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 $MgSiO_4H_2$ phase H has been reported to decompose into H_2O (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_2O 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_2O 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.

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