Effects of hydrogen bond symmetrization on the elastic properties of high pressure polymorphs of ice: ab initio investigation

Jun Tsuchiya[1]; Taku Tsuchiya[2]

[1] GRC, Ehime University; [2] GRC, Ehime Univ

Determination of physical properties and phase relations of high-pressure ice is important for physical, geophysical and planetary sciences. Hydrogen bonded molecular phases ice VIII and ice VII have known to transform to an atomic crystal phase ice X at ˜60-80 GPa. We have reported that the hydrogen bond symmetrization occurs also in hydrous minerals, delta-AlOOH and phase D ($MgSi_2O_6H_2$) at ˜30 and 40 GPa respectively, and it significantly changes their compressibilities, vibrational and elastic properties. Regarding the elastic properties, we have found that some components of elastic constants relating to the hydrogen bonds anomalously increase across the hydrogen bond symmetrization. Such effect of the hydrogen bond symmetrization on elasticity is expected to be observed more prominently in the case of ice, since the ice framework is constructed mainly by the hydrogen bond between H_2O molecules. Here, we investigated by first principles, the elastic properties of high-pressure phases of ice VIII and X.

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