The 435th Geodynamics Seminar

Hydrogen bond symmetrization of ice and hydrous phases

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Abstract

Determination of the structure, 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 ~60-100 GPa by the hydrogen bond symmetrization. We have reported the hydrogen bond symmetrization occurs also in dense hydrous minerals such as δ -AlOOH, phase D (MgSi₂O₆H₂) and phase H (MgSiO₄H₂) at ~ 30 GPa. We have shown that their compressibilities, vibrational and elastic properties are significantly changed by the hydrogen bond symmetrization. Here, I review these behaviors in high pressure ice and hydrous minerals investigated by first principles calculations and compare them with the recent results of the high pressure experiments.