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Venue: Zoom

A link will be sent @grc-all within 30 minutes before the beginning of the seminar.

First principles investigation of high pressure ice phases.

Knowing the structure, physical properties, and phase relations of high-pressure H₂O ice phase 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 by the hydrogen bond symmetrization under pressure. However, the hydrogen dynamics at the transition has not been fully understood so far. We have reported the change of physical properties associated with hydrogen bond symmetrization in high pressure ice and also in dense hydrous minerals such as δ -AlOOH, phase D (MgSi₂O₆H₂) and phase H (MgSiO₄H₂). Here, I review and present the investigation of these behaviors in high pressure ice and hydrous minerals by first principles calculations.

Keywords:

1. Hydrogen bond
2. High pressure
3. First principles calculation