



Dr. Jun Tsuchiya

Associate Professor
Geodynamics Research Center

2022.01.28 (Fri.) 16:30 ~

Venue: Zoom

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

First principles investigations 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. Here, I show the recent our efforts for the understandings of the high-pressure ice phases by first principles calculations.

Keywords:

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