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Dynamical (in)stabilities of high-pressure H2O ices VII, VIII and X RAZVAN CARACAS, CNRS, Ecole Normale Superieure de Lyon — We study high-pressure solid H2O ice: the lattice dynamical properties of ice X and the transition path between molecular ices VII/VIII and the ionic ice X with first-principles calculations using density functional theory in the ABINIT implementation. Our work [PRL 101, 085502] defines the dynamical stability of ice X between about 120 GPa up to about 400 GPa. Based on phonon band dispersion we show that the phase transition sequence at low temperature and high pressures in ice is ice VIII - disordered ice X - ice X - ice Pbcm. The disordered ice X is due to a phonon collapse in the whole Brillouin zone at pressures below 120 GPa, phonon that corresponds to hydrogen atoms bouncing back and forth between every two oxygen neighbors in a double well potential. Post-ice X is orthorhombic Pbcm and appears due to a phonon instability in M at pressures higher than 400 GPa that distorts the bcc cubic sublattice of oxygen atoms into a hcp-like structure. Our calculations validate earlier theoretical predictions for a phase transition to a post-ice X structure in H2O [Benoit et al. PRL 76, 2934]. We also identify and discuss the (meta)stability of several intermediate phases between ice VIII and ice X.

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