**STABILITY OF $H_2O$ ICE POLYMORPHS AT HIGH PRESSURE.** R. Caracas[1] and R.J. Hemley[2], [1]Laboratoire de Sciences de la Terre CNRS UMR5570, Ecole Normale Supérieure de Lyon, 46, allée d'Italie, 69364 Lyon cedex 07, France, razvan.caracas@ens-lyon.fr, [2]Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Brnach Rd., NW, Washington DC 20015, USA, rhemley@ciw.edu

We employ density functional theory as implemented in the ABINIT package [1] to investigate the high-pressure behavior of $H_2O$ ice. We find that at low temperatures ice VII can transform in a metastable tetragonal structure in the same stability field as ice VIII [2]. Ice VIII is thermodynamically stable to at least up 60 GPa. In the 60-120 GPa pressure range we show based on static (0K) and dynamical calculations that disordered ice X is more stable than ice VIII. In this pressure range ice X is characterized by one unstable flat phonon band, which leads to the disordering of the structure. Ice X is dynamically stable above 120 GPa and up to about 400 GPa pressure. In this range, with compression ice X shows a softening of the lowest phonon mode in M (=1/2 1/2 0), which becomes unstable above 400 GPa. The instability corresponds to collective displacements of the hydrogen and oxygen atoms on (110) planes that induce the bending of the O-H-O angle. The structure that results after the lock-in of this unstable mode is the Pbcm orthorhombic structure obtained from molecular-dynamics calculations [3]. Consequently we propose a high-pressure low-temperature phase-transition sequence as ice VIII – disordered ice X - ice X - ice Pbcm.

**References**: [1] Gonze et al., Comp. Mat. Sci. 25, 478 (2002); Z. Kristall. 220, 558 (2005). [2] Maddury et al., J. Chem. Phys., 2007. [3] Benoit et al., Phys. Rev. Lett., 76, 2934, 1996.