Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Order-disorder phase boundary in Ice VII-VIII investigated by first principles** RENATA WENTZCOVITCH, KOICHIRO UMEMOTO, University of Minnesota, STEFANO DE GIRONCOLI, SISSA, STEFANO BARONI, UMN/SISSA COLLABORATION — Phase boundaries among the various forms of ice are difficult to determine experimentally because of large hysteresis involved, especially at the lowest temperatures. Theoretically, there are also great challenges, including the order-disorder (OD) phenomenon. The ice VII-VIII boundary, a typical OD boundary, has been reasonably well constrained experimentally and is an ideal study case. We present a first principles quasiharmonic study consisting in the complete statistical sampling of molecular orientations within a 16-molecules supercell. Our calculation accounts well for several important aspects: equation of state of ice VII, negative Clapeyron slope of the phase boundary, and the isotope effect. We will discuss also some factors to be improved, including XC functionals. Research was supported by NSF grants EAR 0810272, EAR 0635990, ATM 0428774 (VLab), EAR 0757903.

Renata Wentzcovitch
University of Minnesota

Date submitted: 21 Nov 2009 Electronic form version 1.4