

Abstract Submitted
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First principles investigation of the ice VII-VIII (order-disorder) phase boundary KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, STEFANO DE GIRONCOLI, STEFANO BARONI, SISSA & DEMOCRITOS National Simulation Center, Italy — Phase boundaries among the various forms of ice are difficult to determine experimentally because of the large hystereses involved. Theoretically there are also great challenges, including order-disorder (OD). The ice VII-VIII boundary, a typical OD boundary, has been reasonably well constrained experimentally. We present a first principles study consisting in the complete statistical sampling of molecular orientations within a 16 molecules supercell. This supercell size accounts well for several aspects of this transition, including the transition temperature and its pressure dependence in the high P range. The differences at lower Ps are likely to be related with the insufficiencies of DFT, within LDA or GGA, to describe the hydrogen bond. Research supported by NSF/EAR 013533 (COMPRES), 0230319, and NSF/ITR 0428774 (VLab).

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