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**First principles investigation of the ice VII-VIII (order-disorder) phase boundary**<sup>1</sup> RENATA WENTZCOVITCH, KOICHIRO UMEMOTO, MSI and CEMS, University of Minnesota, STEFANO DE GIRONCOLI, STEFANO BARONI, SISSA and DEMOCRITOS National Simulation Center, Trieste, Italy — Phase boundaries among the various forms of ice are difficult to determine experimentally because of the large hystereses involved. Theoretical determination is also very challenging. Treatment of disorder in hydrogen sublattice is one of major problems. We present a first-principles study of order-disorder transition between ice VII and VIII. This study involves the complete statistical sampling of configurations generated within a 16 molecules supercell and includes the important effects of vibrational energy on this phase boundary. Since this transition has been well constrained experimentally, it is a good test of our treatment.

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