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Nuclear Quantum Effects in Different Ice Phases[1] MARIVI FERNANDEZ-SERRA, Stony Brook University, BETUL PAMUK, CNRS and Université Pierre et Marie Curie, PHILIP B. ALLEN, Stony Brook University — We have previously explained that the anomalous isotope effect in hexagonal ices is liked to the anticorrelation between the covalent OH bond and the hydrogen bond by using the quasiharmonic approximation combined with *ab initio* density functional theory. [1] In this study, we show that similar physics plays a role in the isotope effect on temperature of the proton-order/disorder phase transition between ice XI and iceIh. By using a van der Waals density functional, we calculate a temperature difference between heavy and light ices of 6 K as compared to the experimental value of 4 K. [2] Furthermore, we extend our study to analyze the zero-point effects in different ice phases and ice-like structures with different densities and crystal structures to understand how this can be linked to the anomalous isotope effect in liquid water. [3] [1] B. Pamuk, *et al.* Phys. Rev. Lett. **108**, 193003 (2012). [2] B. Pamuk, P. B. Allen, M-V. Fernandez-Serra Phys. Rev. B **92**, 124105 (2015). [3] B. Pamuk, *et al.* in preparation.

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