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Quantum Zero Point Effects in Water and Ice[1] BETÜL PAMUK, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — Nuclear zero point effects have recently been shown to have an interesting quantum anomaly in ice. In particular, In hexagonal ice Ih, the lattice volume increases when H is replaced by D. This anomalous isotope shift of the lattice parameter increases with temperature, contrary to normal expectations [1]. Free energy calculations within the quasiharmonic approximation, with *ab initio* density functional theory, explain the origin of his anomaly. In this study, we extend our study to show that the anomalous isotope effect persists in amorphous ices, inherent structures of liquid water. This indicates that the anomalous isotope effect on the density of liquid water might be intrinsically related to the one observed in ice, even if their structures are radically different. In addition, we show that clathrate hydrides, also have this anomaly. We make a detailed analysis of the origin of the anomaly and study how the Hbond interaction and the vdW bond in liquid water are modified by these nuclear zero point effects. [1] B. Pamuk *et. al*, Phys. Rev. Lett. **108**, 193003 (2012).

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