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Nuclear Zero Point Effects as a Function of Density in Ice-like Structures and Liquid Water from vdW-DF *Ab Initio* Calculations[1]
BETÜL PAMUK, PHILIP B. ALLEN, Stony Brook University, JOSE M. SOLER, Universidad Autonoma de Madrid, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — The contributions of nuclear zero point vibrations to the structures of liquid water and ice are not negligible. Recently, we have explained the source of an anomalous isotope shift in hexagonal ice, representing itself as an increase in the lattice volume when H is replaced by D, by calculating free energy within the quasiharmonic approximation, with *ab initio* density functional theory [1]. In this work, we extend our studies to analyze the zero point effect in other ice-like structures under different densities: clathrate hydrates, LDL and HDL-like amorphous ices with different densities, and a highly dense ice phase, ice VIII. We show that there is a transition from anomalous isotope effect to normal isotope effect as the density increases. We also analyze nuclear zero point effects in liquid water using different vdW-DFs and make connections to this anomalous-normal isotope effect transition in ice. [1] B. Pamuk *et. al*, Phys. Rev. Lett. **108**, 193003 (2012).

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