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Anomalous lattice parameter isotope-shift in hexagonal ice Ih from first principle calculations[1] BETÜL PAMUK, MARIVI FERNANDEZ-SERRA, PHILIP ALLEN, Stony Brook University — The lattice parameters of light (H_2O) and heavy (D_2O) Ih ice differ by 0.09% [1]. The larger lattice constant is that of the heavier isotope, contrary to normal expectations. This isotope shift of the lattice constant is linked to the zero point energy of phonons in ice. In particular, it can be linked to the anti-correlation of the O-H stretch frequency and the O-O distance in H-bonded materials. In order to determine which phonons give the anomaly, we calculate Grüneisen parameters of H_2O and D_2O ice using first principles density functional theory, within the frozen phonon approximation. Our results show a strong dependence on the density functional chosen. We analyze these differences and make connections to experiment. These results indicate that not only H-bond effects but also van der Waals interactions are necessary to reproduce the correct lattice constant zero-point shifts in ice.

[1] B. K. Röttger et. al., Acta Cryst. B **50**, 644-648 (1994).

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