From tetrahedral networks to (meta-) stable ice structures: a theoretical study EDGAR ENGEL, CHRIS PICKARD, RICHARD NEEDS, University of Cambridge, Cambridge, UK, MICHELE CERIOTTI, ANDREA ANELLI, EPFL, Lausanne, Switzerland — We present a comprehensive computational study of the crystalline phases of water ice employing force field and dispersion corrected density functional theory calculations. We construct ice structures on the basis of more than five million tetrahedral networks listed in the Treacy, Deem, and IZA databases and employ the "Sketchmap" dimensionality reduction algorithm of Ceriotti et al. to examine the thus explored configuration space. Assuming no prior knowledge of the known stable phases of water ice, we classify the structures and recover all but two of ices I to XVI and ices i, 0 and the quartz phase of ice. More importantly, we identify them as the most stable representatives of their respective clusters of alike structures. We further identify 10 new dynamically stable structures with competitive enthalpies compared to the know phases of ice. For these we perform anharmonic quantum nuclear vibrational calculations using the VSCF methods of Monserrat et al. We find that two of these structures compare favourably to the theoretical i and 0 phases at similar densities, with one matching the structure recently proposed for ice XVII on the basis of neutron diffraction data.

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