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van der Waals interactions in water and ice from density functional theory simulations: improvements and challenges[1]

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Accounting for long range van der Waals (vdW) type correlations in the description of water and ice has proven to be one of the most important improvements in density functional theory (DFT)-based simulations of water. I will show how our understanding of the network structure in liquid water has changed with the newly available vdW density functionals, derived from the original version of Dion et al. [Phys. Rev. Lett. 92, 246401 (2004)]. In particular I will focus on the links between the density of water and the interplay between the hydrogen bonds and the so called vdW-bonds, easily identifiable in the liquid. These new vdW-DFs have also proven to be very important in the description of ice. In particular I will show how they are capable of accurately describing the anomalous nuclear quantum effects in ice, bringing DFT simulations and experimental results very close together. Our results show that current vdW-DFs are capable of correctly describing the subtle interplay between inter-molecular libration modes and intra-molecular stretching modes in ice, thus reproducing the experimental results once the zero point of these modes is accounted for in the simulations.

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