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The importance of van der Waals dispersion forces in ice B. SANTRA, Fritz-Haber-Institut der MPG, Berlin, A. MICHAELIDES, University College London, London, M. SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — For decades it is known that the condensed phases of water are held together through a combination of hydrogen bonds (HBs) and van der Waals (vdW) dispersion forces. Whilst HBs have received widespread attention, relatively little is known about the importance of vdW forces. Partly this is down to the now most popular electronic structure theory (density-functional theory (DFT)) providing an inadequate description of vdW forces when standard exchange-correlation functionals are used. However, improved semi-empirical vdW corrections to DFT [1] and the non-local vdW functional [2] mean that it is now possible to shed light on this issue. Here, we report simulations on a range of ambient and high pressure phases of ice to understand the delicate interplay of HBs and vdW. We find that the proportion of the lattice energy coming from vdW forces monotonously increases as the density of the ice phases increases, and as a consequence vdW plays a crucial role in determining the relative stabilities of the high density phases of ice. In addition, our calculations show that the effective volume of the water molecules is reduced when vdW is accounted for and provide general insights into the importance of vdW forces in other condensed phases of water. [1] Tkatchenko *et al.*, PRL **102**, 073005 (2009), [2] Dion *et al.*, PRL **92**, 246401 (2004).

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