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Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures BISWAJIT SANTRA, Fritz-Haber-Institut der Max-Planck-Gesselschaft, Berlin, Germany, JIŘÍ KLIMEŠ, London Centre for Nanotechnology and Department of Chemistry, University College London, London, UK, DARIO ALFÈ, Department of Earth Sciences, University College London, London, UK, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesselschaft, Berlin, Germany, BEN SLATER, Department of Chemistry, University College London, London, UK, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, London, UK, ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesselschaft, Berlin, Germany

— The balance between van der Waals (vdW) forces and hydrogen bonding in ambient and high pressure phases of ice has been examined with the first principles approaches, density-functional theory (DFT) and quantum Monte Carlo. At higher pressure, the contribution to the lattice energy from vdW increases and that from hydrogen bonding decreases, leading vdW to have a substantial effect on the transition pressures between the crystalline ice phases. An important consequence, likely to be of relevance to molecular crystals in general, is that the transition pressures obtained from DFT functionals which neglect vdW forces are greatly overestimated [Phys. Rev. Lett. **107**, 185701 (2011)].

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