Abstract Submitted
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**Van der Waals interactions and vibrational effects in ice from first principles**[1] EAMONN MURRAY, GIULIA GALLI, University of California, Davis
— We present a comparative study of the equation of state and of the electronic and vibrational properties of ice XI and VIII, as obtained with ab-initio calculations using semi-local (PBE) and nonlocal, van der Waals functionals. The two functionals yield similar electronic properties for both phases, however they perform very differently in describing their vibrational properties, and the transition pressure from the low to the high pressure phase. The latter is overestimated by a factor of about 6 when using PBE and in agreement with experiment when dispersion forces are taken into account. The inclusion of zero point energy contributions does not affect the computed transition pressure, while it substantially affects structural properties, including equilibrium volumes and bulk moduli, especially for the high pressure phase.

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