

Abstract Submitted  
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**Ice under pressure: the role of van der Waals forces in hydrogen bonding**<sup>1</sup> EAMONN MURRAY, GIULIA GALLI, UC Davis — We will discuss the evolution of the role of van der Waals interactions in hydrogen bonding in high pressure phases of ice. Here, we compare first principles results of the structural and electronic properties of ice using several different approaches to the calculation of exchange and correlation energies. These include the non-local vdW density functional of Dion *et al*<sup>2</sup>, the revised vdW density functional of Lee *et al*<sup>3</sup> and the EXX/RPA approach based on an eigenvalue representation of the dielectric matrix<sup>4</sup> along with the semilocal functional PBE and hybrid functional PBE0.

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<sup>3</sup>K. Lee, É. D. Murray, L. Kong, B. I. Lundqvist and D. C. Langreth, Phys. Rev. B **82**, 081101 (2010)

<sup>4</sup>D. Lu, Y. Li, D. Rocca and G. Galli, Phys. Rev. Lett. **102**, 206411 (2009)

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