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To wet or not to wet? Dispersion forces tip the balance for water ice on metals JAVIER CARRASCO, Instituto de Catalisis y Petroleoquimica, CSIC, Marie Curie 2, E-29049 Madrid, Spain, BISWA-JIT SANTRA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, JIRI KLIMES, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, UK – For almost 30 years now, density functional theory (DFT) has been used to explore the molecular level details of water-metal interfaces. However, since the typical generalized gradient approximation exchangecorrelation functionals used in these studies do not account for van der Waals (vdW) dispersion forces, the role dispersion plays in water adsorption remains unclear. Here, we tackle this issue head on applying a newly developed non-local functional [J. Klimeš et al., J. Phys.: Condens. Matter 22, 022201 (2010)] to two of the most widely studied water-ice adsorption systems, namely water on Cu(110) and Ru(0001). We show that non-local correlations contribute substantially to the water-metal bond and that this is an important factor in governing the relative stabilities of wetting layers and 3D bulk ice [J. Carrasco *et al.*, Phys. Rev. Lett. **106**, 026101 (2011)]. Due to the greater polarizability of the substrate metal atoms, non-local correlations between water and the metal exceed those between water within ice. This sheds light on a long-standing problem, wherein common DFT exchange-correlation functionals incorrectly predict that none of the low temperature experimentally characterized Javier Carrasco ice-like wetting layers are thermodynamically stable. Javier Carrasco Instituto de Catalisis y Petroleoquimica, CSIC, Marie Curie 2, E-29049 Madrid, Spain

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