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Quantum nature of the proton in water-hydroxyl overlayers on metal surfaces ANGELOS MICHAELIDES, XINZHENG LI, London Centre for Nanotechnology and Department of Chemistry, University College London, MATTHEW PROBERT, Department of Physics, University of York, ALI ALAVI, Department of Chemistry, University of Cambridge — Using *ab initio* path integral molecular dynamics we show that water-hydroxyl overlayers on transition metal surfaces exhibit surprisingly pronounced quantum nuclear effects. The metal substrates serve to reduce the classical proton transfer barriers within the overlayers and, in analogy to ice under high pressure, to shorten the corresponding intermolecular hydrogen bonds. Depending on the substrate and the intermolecular separations it imposes, the traditional distinction between covalent and hydrogen bonds is lost partially (e.g. on Pt(111) and Ru(0001)) or almost entirely (e.g. on Ni(111)). We suggest that these systems provide an excellent platform on which to systematically explore the magnitude of quantum nuclear effects in hydrogen bonds.

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