

Abstract Submitted
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Quantum nature of protons in water probed by scanning tunneling microscopy and spectroscopy JING GUO, Peking Univ, JING-TAO L, Huazhong University of Science and Technology, YEXIN FENG, Hunan University, JI CHEN, University College London, JINBO PENG, ZEREN LIN, XIANGZHI MENG, ZHICHANG WANG, XIN-ZHENG LI, EN-GE WANG, YING JIANG, Peking Univ, JING-TAO L TEAM, XIN-ZHENG LI TEAM — The complexity of hydrogen-bonding interaction largely arises from the quantum nature of light hydrogen nuclei, which has remained elusive for decades. Here we report the direct assessment of nuclear quantum effects on the strength of a single hydrogen bond formed at a water-salt interface, using tip-enhanced inelastic electron tunneling spectroscopy (IETS) based on a low-temperature scanning tunneling microscope (STM) [1]. The IETS signals are resonantly enhanced by gating the frontier orbitals of water via a chlorine-terminated STM tip, such that the hydrogen-bonding strength can be determined with unprecedentedly high accuracy from the redshift in the O-H stretching frequency of water. Isotopic substitution experiments combined with quantum simulations reveal that the anharmonic quantum fluctuations of hydrogen nuclei weaken the weak hydrogen bonds and strengthen the relatively strong ones. However, this trend can be completely reversed when the hydrogen bond is strongly coupled to the polar atomic sites of the surface. References: [1] J. Guo *et al.* Science. 352321 (2016).

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