复旦大学物理系物质科学报告

Physics Department Colloquium

Probing quantum nature of hydrogen bond with scanning tunneling microscopy and spectroscopy

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Abstract: It has been known that the complexity of hydrogen-bonding interaction largely arises from the quantum nature of light hydrogen nuclei (proton). The so-called nuclear quantum effects (NQEs) in terms of tunneling and zero-point motion play important roles in the structure, dynamics, and macroscopic properties of hydrogen-boned materials. Despite enormous theoretical efforts on pursuing proper treatment of the nuclear motion at a quantum-mechanical level, accurate and quantitative description of NQEs on the hydrogen-bonding interaction has proven experimentally challenging. In this talk, I will present our recent progresses on probing NQEs of interfacial water at single bond limit using a low-temperature scanning tunneling microscope (STM). By gating the molecular frontier orbitals near the Fermi level via tip-water coupling, we are able to access the internal degrees of freedom of water molecules and locate the protons in real space [1,2]. These techniques allow us not only to directly visualize the many-body proton tunneling within the H-bonded network [3], but also to quantify the impact of nuclear quantum fluctuation on the strength of hydrogen bonds [4]. Our work opens up the possibility of directly assessing, in experiment, the impact of NQEs on hydrogen-bonding interaction, which is essential for elucidating the quantum nature of the hydrogen bonds.

[1] J. Guo *et al*., Nature Materials **13**, 184 (2014).
[2] J. Chen *et al*., Nature Communications **5**, 4056 (2014).
[3] X. Meng *et al*., Nature Physics **11**, 235 (2015).
[4] J. Guo *et al*., *to be submitted.*

Time：2:00pm, Tuesday, April 21, 2015

Location：Physics Building, Room 221B

(Cookies and coffee will be served from 1:30 pm)