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Tenkých vrstev a nanostruktur

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TÉMA

Direct observation and control of H-bond dynamics using scanning probe microscopy

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H-bond dynamics is involved in many chemical and biological processes, and has been intensively studied by multiple experimental and theoretical methods [1]. In particular, rotational–vibrational spectroscopy and quantum chemical calculations have greatly contributed to revealing the fundamental aspects. However, direct observation and control of H-bond dynamics were rarely reported at the single-molecule level. A majority of chemical and biological processes take place in condensed phases where impact from the local environment, which causes static or dynamic perturbation on the process, plays a crucial role; it is therefore important to study the dynamics with individual molecules. Additionally, for H-bond dynamics, quantum nuclear effects (QNEs) become pronounced and govern the process in some cases due to the small mass of H atom. The accurate description of QNEs in complex multidimensional potential energy surfaces – this is particularly the case for reactions in condensed phases – remains a challenging problem.

I will discuss the direct observation and control of H-bond dynamics using low-temperature scanning tunneling and atomic force microscopy and present H-bond exchange reaction governed by tunneling within a water dimer [2], vibrationally-induced H-atom relay reactions within water–hydroxyl complexes [3], and STM-/atomic force-induced intramolecular H-atom transfer reaction (tautomerization) within a porphycene molecule [4]. These results provide novel insight into H-bond dynamics at the single-molecule level and unveil impact from the local environment on the process. Our approach opens up a new opportunity of studying physical chemistry at the bottom [5].

References:

[1] J. T. Hynes, J. P. Klinman, H.-H Limbach, R. L. Schowen, Hydrogen-transfer reaction, Viley-VCH. **[2]** T.K. et al. Phys. Rev. Lett. 100, 166101 (2008). **[3]** T.K. et al. Nat. Mater. 11, 167 (2012). **[4]** T.K. et al. Phys. Rev. Lett. 111, 246101 (2013).; T.K. et al. Nat. Chem. 6, 41 (2014). **[5]** T.K. Visualization of hydrogen-bond dynamics, Springer Theses 125. Springer Verlag, 2012.; T.K. Prog. Surf. Sci. 90, 239 (2015).

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