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Physical Chemistry with Single Molecules—Hydrogen-Transfer Dynamics Studied by Scanning Probe Microscopy

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H-atom transfer and H-bond rearrangement are involved in many important physical, chemical, and biological processes such as proton conductor, acid-base reactions, and DNA [1]. However, an accurate and quantitative description of H-atom/bonding dynamics remains a very challenging topic and nuclear quantum effects (NQEs) and anharmonicity of the potential energy surface are outstanding problems in the field. In order to examine such dynamics, it is necessary to investigate model systems at the single-molecule level because NQEs and anharmonic nature are quite susceptive to a local environment of individual molecules and hidden by inhomogeneities of bulk samples. Low-temperature SPM has provided a new opportunity to study hydrogen-atom/bonding dynamics [2]. Single-molecule tautomerization serves as a fascinating model and I will discuss hydrogen-transfer reactions occurring through various external stimuli as well as quantum tunneling [3].

## References

[1] Hydrogen-transfer reaction. J. T. Hynes, J. P. Klinman, H.-H. Limbach, R. L. Schowen, Weley-VCH, 2007.

[2] TK, Prog. Surf. Sci. 90, 239 (2015).

[3] TK et al. Phys. Rev. Lett. 111, 246101 (2013).; TK et al. Nature Chem. 6, 41 (2014).; J. Ladenthin et al. ACS Nano 9, 7287 (2015).; H. Böckmann et al. Nano Lett. 16, 1034 (2016).; J. Ladenthin et al. Nature Chem. 8, 935 (2016).; M. Koch et al. J. Am. Chem. Soc. 139, 12681 (2017).; TK, J. Chem. Phys. 148, 102330 (2018):; H. Böckmann et al. Nano Lett. 18, 152 (2018).

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