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Following elemental chemical steps by imaging molecular orbitals by STM[1]

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Probing the electronic structure of molecules by STM is complicated by the strong interaction of the molecular orbitals with the metal substrate.[1,2] Adsorbing the molecule on an ultrathin insulating film alleviates this problem and allows direct imaging of molecular orbitals in real space.[1] This approach will be illustrated by two examples: characterizing the operation of a single-molecule switch and controlling and monitoring the formation of an organometallic complex. The inner hydrogens in the central cavity of a naphthalocyanine molecule can be switched between two equivalent positions.[3] This process (hydrogen tautomerization reaction) can be initiated in a controlled fashion by excitation induced by the inelastic tunnelling current. The tautomerization reaction can be followed by resonant tunnelling through the LUMO of the molecule and is expressed as considerable changes in the conductivity. In addition, we demonstrate a coupling of the switching process so that the charge injection in one molecule induces tautomerization in an adjacent molecule. The other example will consider constructing an organometallic complex from individual organic molecules and metal atoms by STM manipulation on the ultrathin insulating film. The manipulation process and the associated changes in the molecular orbitals (energy, spatial extension, symmetry) can be followed STM imaging and spectroscopy.

[1] J. Repp et al. Phys. Rev. Lett. 94, 026803 (2005).
[2] X.H. Qiu, G.V. Nazin, W. Ho Science 299, 542 (2003).
[3] P. Liljeroth, J. Repp, G. Meyer Science 317, 1203 (2007).

[1]Work in collaboration with Jascha Repp and Gerhard Meyer.