

# Single-Molecule Isomerization—A Novel Tool for Probing Quantum-Mechanical Interference Effects

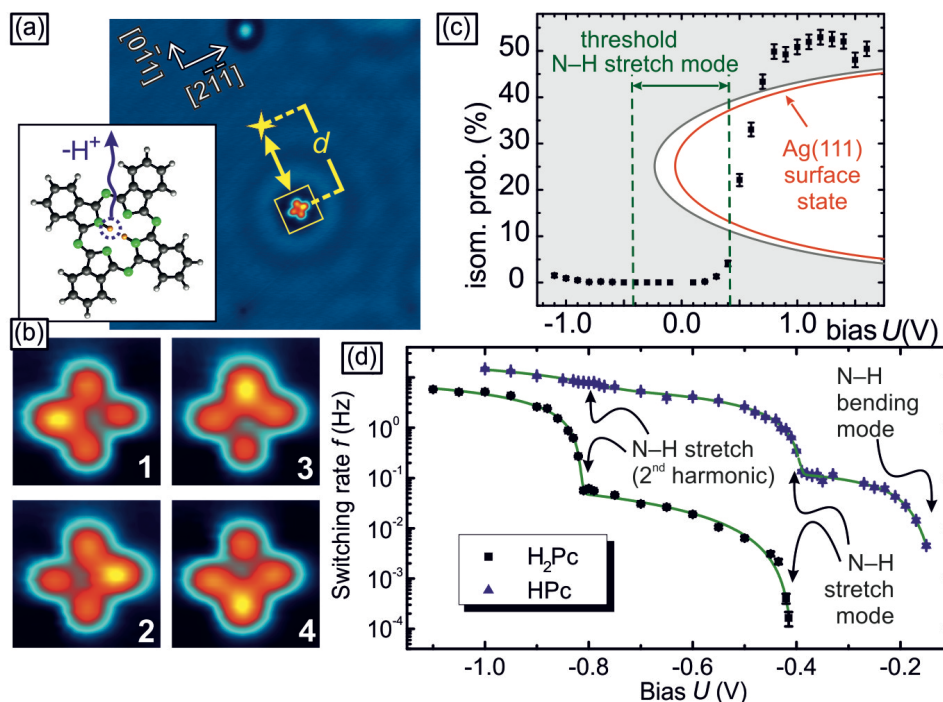
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It is known for quite a while that charge currents between the tip of a scanning tunnelling microscope (STM) and a molecule can induce molecule isomerization, i.e., the molecule maintains its chemical formula but changes its structure. For example, the hydrogen atom in the centre of the HPc molecule can occupy four different positions. Whereas usually performed with the STM tip positioned directly over the molecule, recent experiments demonstrated remote STM-induced isomerization, where isomerization is triggered by charge carriers injected at a distance of several nanometers from the molecule. The detailed processes responsible for nonlocal switching are largely unknown.

In my talk I will demonstrate for phthalocyanine molecules on Ag(111) how the of nonlocal, hot electron-induced tautomerization rate can controllably be decreased or increased by Ag nanostructures. For example, walls constructed from single Ag atoms act as potential barriers that exponentially damp the hot electron current. Conversely, by using elliptical nanostructures, we can coherently focus them onto the molecule.

Bias-dependent experiments reveal how the quasiparticle transport proceeds. For example, the surface electronic structure of Ag(111) is dominated by an electron-like surface state. Electrons which tunnel into this surface state propagate to the molecule where they induce isomerization via inelastic processes (in this case the N–H vibrational stretch mode). In contrast, the probability that bulk electrons reach the molecule is extremely low since the majority recombines in the bulk. In an outlook, I will discuss the potential of this method to measure transport properties on the 10 nm-scale.



**Fig.** (a) STM image of HPc/Ag(111) (inset: schematic HPc structure). (b) STM images of four HPc isomers. (c) Bias-dependent STM-induced isomerization probability of HPc on Ag(111) (background: dispersion of the Ag(111) surface state (red) and surface-projected bulk band structure (grey)). (d) Bias dependence of the switching rate  $f$  of HPc and H<sub>2</sub>Pc. Various inelastic modes can be recognized by a steep rise in  $f$ . All data taken at  $T = 5$  K.