Scanning Probe Microscopy of Adsorbates on Insulating Films: First Steps towards a modular molecular logic

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Ultrathin insulating films on metal substrates are unique systems to use the scanning tunneling microscope to study the electronic properties of single atoms and molecules, which are electronically decoupled from the metallic substrate.

Individual gold atoms on an ultrathin insulating sodium chloride film supported by a copper surface exhibit two different charge states, which are stabilized by the large ionic polarizability of the film [1]. The charge state and associated physical and chemical properties such as diffusion can be controlled by adding or removing a single electron to or from the adatom with a scanning tunneling microscope tip. The simple physical mechanism behind the charge bistability in this case suggests that this is a common phenomenon for adsorbates on polar insulating films. For example in the particular case of Ag adatoms even three different charge states could be observed [2].

In the case of molecules on ultrathin NaCl films the electronic decoupling allows the direct imaging of the unperturbed molecular orbitals. This will be shown for individual pentacene molecules [3]. Scanning tunneling spectroscopy of these double-barrier tunneling-junctions reveals strong electron-phonon coupling to NaCl phonons.

Using atomic/molecular manipulation a covalent bond between an individual pentacene molecule and a gold atom can be formed. This bond formation is reversible and different structural isomers can be produced. Direct imaging of the orbital hybridization upon bond formation provides insight into the energetic shifts and occupation of the molecular resonances.

Molecular switches will be an essential part of possible future molecular devices. The bistability in the position of the two hydrogens in the inner cavity of single free-base naphthalocyanine molecules (Fig.1) constitutes a two-level system that can be manipulated and probed by low-temperature scanning tunnelling microscopy. When adsorbed on an ultrathin insulating film, the molecules can be switched in a controlled fashion between the two states by excitation induced by the inelastic tunnelling current. The tautomerization reaction can be probed by resonant tunnelling through the molecular orbitals (Fig. 2). Coupling of the switching process such that charge injection in one molecule induced tautomerization in an adjacent molecule will be shown.

References

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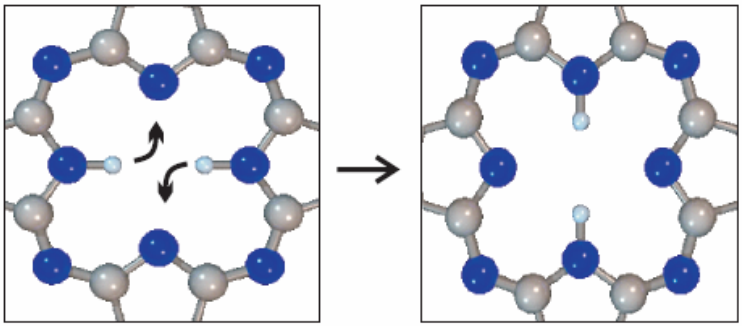

Fig. 1 Model of hydrogen tautomerization in the inner cavity of a naphthalocyanine molecule

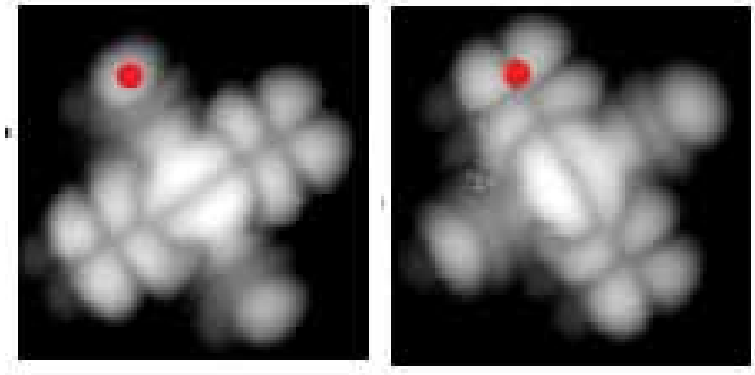

Fig. 2 Switching between the two configurations as imaged directly by the orientation of the LUMO of the naphthalocyanine molecule.