

Scanning Tunneling Spectroscopy and Atomic Force Microscopy of Individual Molecules on Thin Insulating Films

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

The ionic relaxations in a polar insulator lead to a charge bi-stability in some adsorbed atoms and molecules. It is shown that control over the charge-state of individual molecules in such systems can be obtained by choosing a substrate system with an appropriate work function. We study the spatial distribution of the additional charge by suitable subtraction of low-voltage STM images of the adsorbates in their different charge states. These difference images show marked intra-molecular contrast [1].

We studied the same system by means of atomic force-microscopy (AFM) in a combined STM/AFM based on the qPlus-sensor [2]. We again produced difference images from subtracting two constant-height Δf -images of the molecule in both charge states. Also these AFM difference images show marked intra-molecular contrast that can be rationalized as being due to vertical relaxations of the molecule upon charging.

In addition, we investigated $C_{20}S_2H_{12}$ molecules adsorbed on ultrathin layers of NaCl in our combined STM/AFM setup. These non-planar molecules exist in two stable conformations. By means of excitations from inelastic tunneling electrons we can switch between both conformations. We present atomic force microscopy (AFM) measurements with submolecular resolution directly revealing the conformational changes [3].

From AFM data and taking the chirality of the molecules into account, we could unambiguously determine the pathway of the conformational change. Hence, the AFM channel reveals additional information that is truly complementary to the STM data set.

Finally, we formed artificial metal-organic complexes on the same substrate by means of inelastic excitations. The electronic decoupling of the ultrathin NaCl films enabled the study of the molecular electronic structure of the constituents and the complex by means of scanning tunnelling spectroscopy. The actual bonding geometry was determined from AFM images with submolecular resolution. Exploiting the symmetry of the complex its electronic structure can be rationalized from considering the linear combinations of the constituents' orbitals.

References

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