

Charge distribution of a single CuPc molecule on NaCl and Cu(111)

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Molecule-substrate interactions inherently influence the performance of organic-based devices. Because molecules of interest are extended objects possessing several vibrational, conformational, and orientational degrees of freedom, adsorption tip-induced rearrangements can be rather complex. [1-3] The adsorption geometry is a crucial factor not only in molecular diffusion and self-assembly, but can also significantly influence the electronic properties of the combined system.

We present low-temperature tuning fork based measurements of the tunneling current and the frequency shift as a function of distance or lateral position and the applied bias voltage of individual copper phthalocyanine (CuPc) molecules. Outside the range where telegraph current noise is detected [3], a bias dependent hysteretic contrast transition between different configurations was observed for CuPc molecules on a bare Cu(111) surface. Supported by first principles calculations, this transition can be attributed to a rotation of the molecules around its center from a twofold symmetric to one of two equivalent distorted configurations.

Furthermore, the influence on the submolecular electronic charge redistribution due to different substrates has been investigated by a comparison of constant tunneling current [see Fig. 1] and constant height current and frequency shift images and spectra recorded on Cu(111) substrates with and without an intervening epitaxial NaCl(001) bilayer. Local potential variations measured by Kelvin probe force spectroscopy showed a much weaker corrugation than in the presence of the NaCl layer. Density functional theory calculations elucidate adsorption-induced structural deformations of the molecule and provide additional insights into observed STM [3,4] and KPFM images.

Support from the Swiss National Science Foundation, the Polish-Swiss Research project PSPB-085/2010 and from PRESTO-JST is acknowledged.

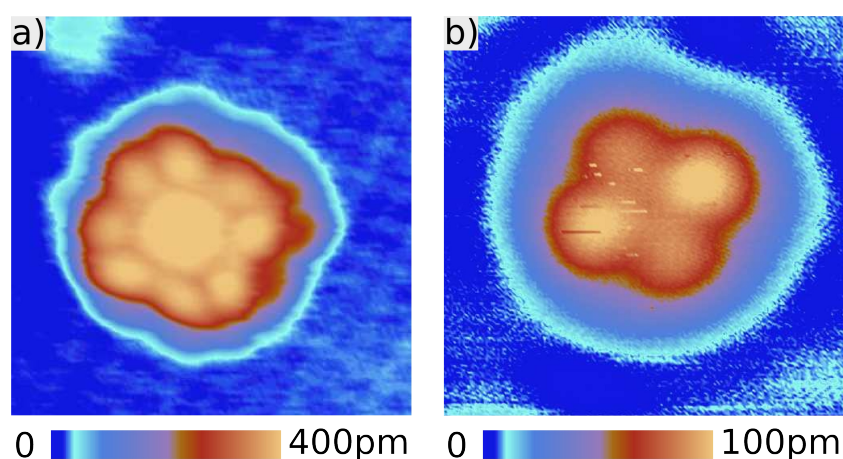


Fig 1: STM images of CuPc on NaCl/Cu(111) (a) and on Cu(111)(b).

References:

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