Arrangement and electronic properties of cobalt phthalocyanine molecules on B-Si(111)-$\sqrt{3} \times \sqrt{3}$ *R* 30°

S. Lindner,[1] M. Franz,[1] M. Kubicki,[1] S. Appelfeller,[1] M. Dähne,[1] and H. Eisele[1]

[1] *Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany*

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject, both from the viewpoint of basic science and in regard of applications. Transition metal phthalocyanines represent a family of organic semiconductors, which are based on a π-conjugated macrocycle ring. Cobalt phthalocyanine (CoPc) is an interesting candidate for interface research, due to its partially filled d_{z2} orbital.

However, the combination of transition metal phthalocyanines with the existing microelectronics technology, being predominantly silicon based, has the potential of novel applications as semiconductor devices. Moreover, semiconductor substrates offer the possibility to tune the molecule substrate interaction by a passivation of the surface. A prominent example in this case is the B-Si(111)-$\sqrt{3} \times \sqrt{3}$ *R*30° (Si:B) surface. The incorporation of B atoms in the subsurface layer leads to a removal of the dangling bonds of the Si(111) surface. This results in an empty p_z orbital of the Si adatom and a chemical deactivation of the surface.

In this talk we demonstrate the molecular arrangement and electronic properties of CoPc on the deactivated Si:B surface in detail by means of scanning tunneling microscopy (STM) as well as spectroscopy (STS). Our data clearly show that submonolayers of CoPc lie flat on the surface and that a selective orbital hybridization occurs. Furthermore, our photoemission spectroscopy (PES) data support the model of the formation of local hybrid state between the partially filled d_{z2} orbital of the CoPc molecule and the empty p_z orbital of the Si adatom. For high CoPc coverages, in contrast, CoPc molecules are tilted with respect to the Si:B surface establishing exceedingly ordered molecular arrangements. The spectroscopic data show clearly that several monolayers of CoPc feature identical electronic properties as pure CoPc.

Financial support by the Deutsche Forschungsgemeinschaft of Project No. LI 3068/2-1 is gratefully acknowledged.

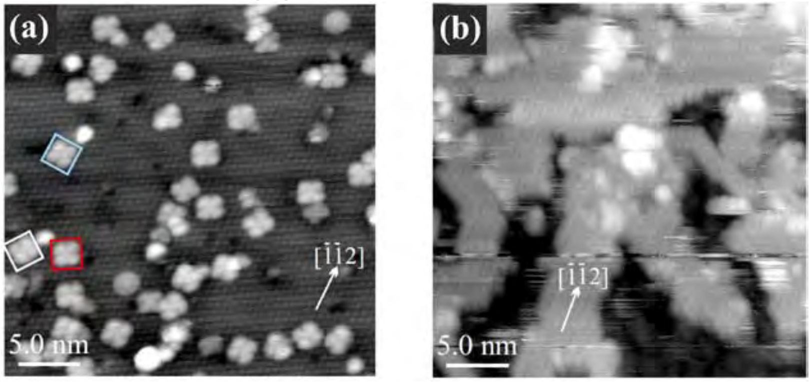

Figure 1. (a) Empty states STM image of a passivated Si:B substrate with a CoPc coverage of 0.2 ML (sample voltage V_S =+1.8 V, tunneling current I_T =50 pA). The different molecular orientations are indicated by colored squares. (b) Empty states STM image of a Si:B surface with a CoPc coverage of 3.2ML (V_S =+2.5 V, I_T =20 pA)

Suplementary Pages

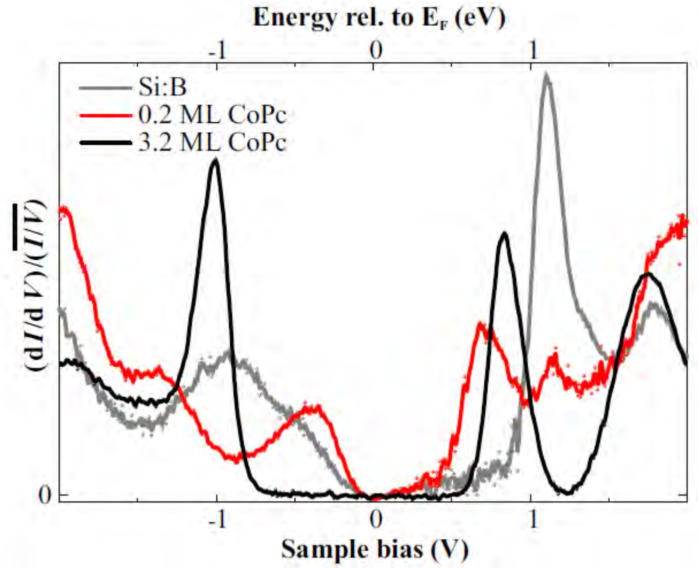

Figure 2: STS results of the normalized differential conductivity of the bare Si:B substrate and with different CoPc coverages. The LDOS spectrum of a 0.2 ML thick CoPc film (red line) shows a very different appearance. A new peak appears at -0.4 V at the valence band side. This occupied state is induced by a charge transfer between the Co atom and the Si:B surface resulting in a reduced electron density at the Co atom.

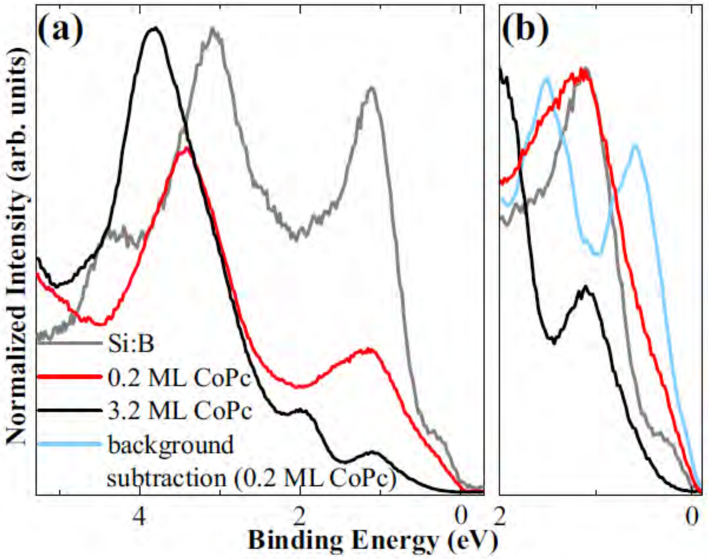

Figure 3: (a) Valence band spectra of CoPc adsorbed on a Si:B surface with increasing film thickness, taken with a photon energy of hν = 62 eV. (b) A close up view of the low binding energy range showing the result of the subtraction of the Si related background from the spectrum of 0.2 ML CoPc as light blue line.