Arrangement and electronic properties of cobalt phthalocyanine molecules on B-Si(111)-√3 × √3 R30°

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Cobalt phthalocyanine (CoPc) is an interesting planar organic semiconductor for functionalized interfaces due to its partially filled central d_{z^2} -orbital. Especially, on passivated semiconductor surfaces the control with the molecular interaction is possible. For this purpose, the B-Si(111)-√3 × √3 R30° (Si:B) surface is used as a model system for the deposition of CoPc.

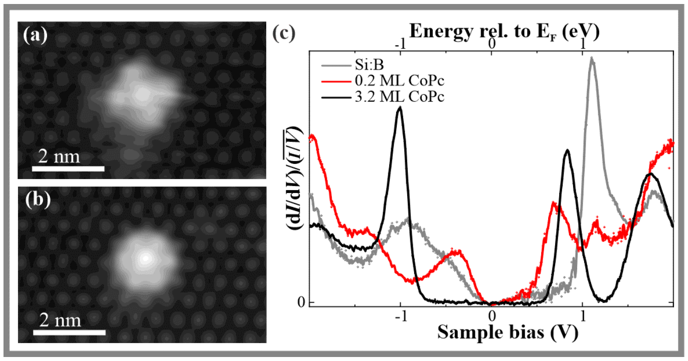

Fig. 1. Empty-state STM images of single flat-lying CoPc molecules (V_S = +2.5 V, I_T = 50 pA) with (a) cloverlike and (b) circular shape. In (c), STS results of the normalized differential conductivity of the bare Si:B substrate and with different CoPc coverages.

In this contribution, we investigate the molecular arrangement and electronic properties of CoPc on the passivated Si:B surface in detail by means of scanning tunneling microscopy (STM) as well as tunneling (STS) and photoemission spectroscopy (PES) [1-3]. The STM images in Fig. 1 clearly show that submonolayers of CoPc lie flat on the surface, with either a four-leaf cloverlike (a) or a circular (b) appearance, depending on the presence of neighboring molecules or surface defects, which affect the molecular rotation, and that a selective orbital hybridization occurs (Fig. 1c). Furthermore, PES data explain that the spectral changes are mostly related to the chemical interactions, while the previously discussed changes of the band bending only play a minor role [3].

For high CoPc coverages, in contrast, the molecules are tilted with respect to the Si:B surface, establishing exceedingly ordered molecular arrangements. The STS data in Fig. 1c (black line) show that several monolayer thick films of CoPc exhibit identical electronic properties as compared with pure CoPc.

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