Growth and Electronic Structure of Conjugated Molecules on Patterned Substrates

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Conjugated molecules being the active material in organic electronic and optoelectronic devices are often elongated structures. As a consequence, key properties such as light absorption/emission or charge transfer ability are also highly anisotropic. To optimize device performance, it is often wanted that the organic is in crystalline order or at least possesses a preferred alignment. This can be achieved by growth on patterned single crystal substrates such as pristine Cu(110) or the Cu(110)-p(2x1)O reconstructed surface, which are of twofold symmetry.

Furthermore, we predict future organic electronic and optoelectronic devices and sensors to be based on lateral structures with length scales of larger conjugated molecules. Such structures can be envisaged to be produced by top down lithographic approaches, or they can be created via bottom up molecular self organisation. An interesting nanoscopically patterned template for growing molecular nanostructures is the Cu(110)-p(2x1)-O reconstructed stripe phase, which consists of alternating stripes of clean Cu(110) and Cu-O with a periodicity in the few nanometer range (Fig. 1a).

The presented results first include the adsorption of heptacene (7A) on Cu(110) versus Cu(110)-(2x1)-O which has been studied with photoemission orbital tomography (POT), scanning tunneling microscopy (STM) and density functional calculations to demonstrate the influence of surface passivation on the molecular geometry and electronic states. The charge transfer into the 7A molecules observed on Cu(110) is completely suppressed for the oxygen-modified Cu surface and the molecules are aligned along the Cu-O rows. They adsorb tilted due to the geometry enforced by the substrate and the ability to maximize intermolecular π-π overlap, which leads to strong π-band dispersion as shown by POT (Fig. 1 b). Second, the nanoscopically patterned Cu-O stripe phase was used as a growth template for 7A, where the molecular length is approximately that of the stripe pattern. We resolve the geometric and electronic alignment of 7A on this nanoscopically confined system to the two pure surfaces above. The results show that despite their small dimensions, the stripes retain the properties of the original surfaces upon 7A adsorption. This produces an array of alternating stripes occupied with neutral and more than doubly charged 7A molecules.

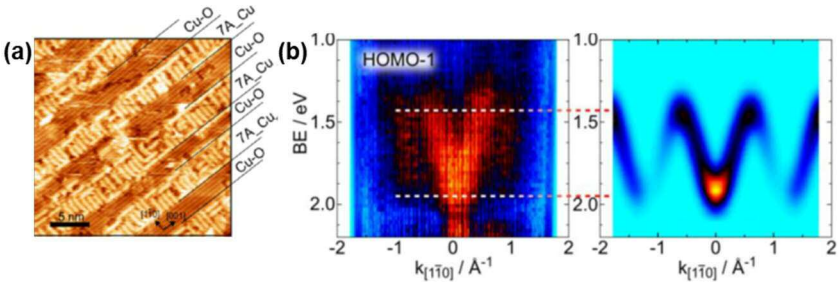

Fig 1 (a) STM measurements of 0.5 ML 7A on the Cu(110) and Cu(2x1)O 50% stripe phase, the respective areas are indicated. (b) Experimental and theoretical band maps (E vs kx) of the 7A on Cu(2x1)O HOMO-1 band at ky = 1.0 Å^{-1}. The simulated band maps have been broadened by 50 meV, and the lateral shift between neighbouring molecules is that suggested from the STM results.

Finally, an outlook to the recently started FWF-WEAVE project: “Longer Acenes: Synthesis, Interface Formation and Thin Film Stability” will be given.