Investigation of adsorption geometries of single Cu-TCPP on rutile TiO₂ (110)

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Molecular adsorbates on surfaces play a major role in many new emerging technologies like hybrid photovoltaics or catalysis. For these applications the adsorption geometry of the molecule is crucial since it influences the electronic properties at the interface, which in turn determines the performance of devices. In many applications like e.g. dye-sensitized solar cells titanium dioxide is widely used as substrate. Hence, the rutile TiO_2 (110) structure of titania has become a model system. Due to their tuneability, porphyrins and phthalocyanines are often used as adsorbates.

In this study we investigate the adsorption geometry of single copper porphyrins (Cu-TCPP) on rutile TiO_2 (110) in UHV. In order to determine the adsorption sites and configuration, we applied noncontact atomic force microscopy (nc-AFM) and Kelvin probe force microscopy (KPFM) as well as scanning tunnelling microscopy (STM) at low temperature. Different adsorption geometries have been observed with nc-AFM. We find that the molecules lie flat on the surface and do not necessarily bind covalently to the surface. The adsorption geometries were further confirmed by high resolution STM. KPFM measurements reveal a work function difference between the adsorbates and the bare substrate. Particularly we observe that heat treatment of the covered surface leads to a strongly, most probably covalently, bound molecule.