

## Interaction of Metallo-Carboxyphenyl Porphyrins with Rutile and Anatase TiO<sub>2</sub>

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Dye-sensitized titanium dioxide is of great interest for photocatalysis and photovoltaics. The structure of the deposited monolayer and the configuration of the single molecules within such layers are of great importance for the device performance. It is therefore necessary to understand the sensitization process and the interaction of single molecules with the surface and among the molecules. In our work we focused mainly on the interaction of single metallo-carboxyphenyl porphyrins with the rutile (110) and anatase (101) surfaces. In order to assess the adsorption configurations of different porphyrins and their electrical properties, we used scanning probe methods such as scanning tunneling, atomic force and Kelvin probe force microscopy as well as photoelectron spectroscopy. On rutile (110) the evaporated porphyrins aligned themselves with respect to the bridging oxygen rows on the surface, resulting in two main orientations, as e.g. depicted for Cu-TCPP in Figure 1. Further investigation of the anchoring revealed that the porphyrins only bind covalently through their carboxylic group if induced by heating during or after deposition. Similar experiments were also performed on the anatase TiO<sub>2</sub> (101) surface, which is even more relevant for the applications. There we found that, even though the surface structure is similar, the porphyrins did hardly bind to the terraces but rather stuck to the step edges. However, formation of covalent bonds to the terraces was also achieved by heating of the substrate during deposition. The results from our research are critically discussed with respect to the application of the sensitizers in dye-sensitized solar cells.

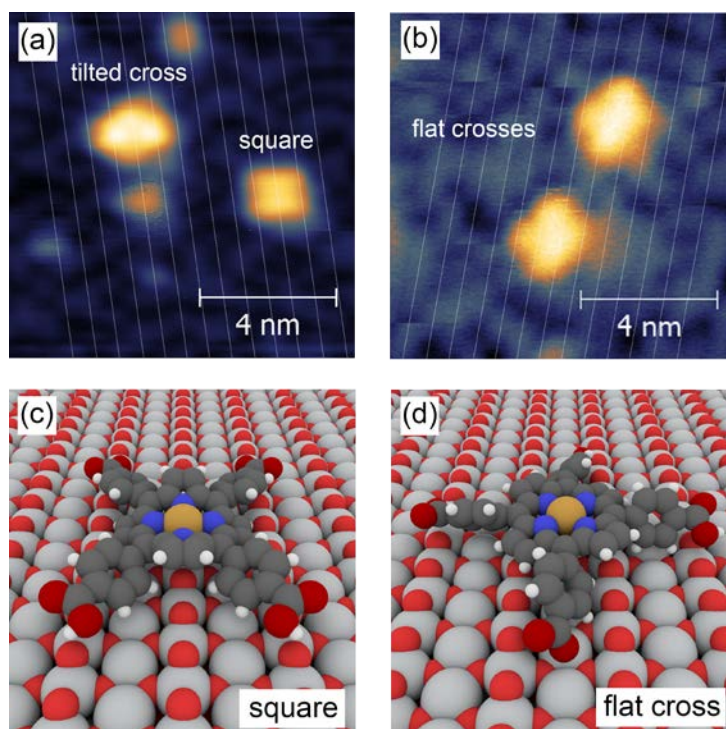


Fig1. Adsorption configurations of Cu(II) tetrakis(4-carboxyphenyl)porphyrin on rutile (110): (a) and (b) atomic force microscopy images, (c) and (d) suggested adsorption mode for two of the orientations shown in (a) and (b).

1. R. Jöhr et al., *The Journal of Chemical Physics* **143**, 094202 (2015).

**Presentation Method (Poster/ Invited Oral 15/20/25/30minutes): Invited 20 (+5) minutes**

**Preferred workshop: Fundamental Properties Investigation of Titanium Oxides**