Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interfacial Interactions between CoTPP Molecules and MgO(100) Thin Films

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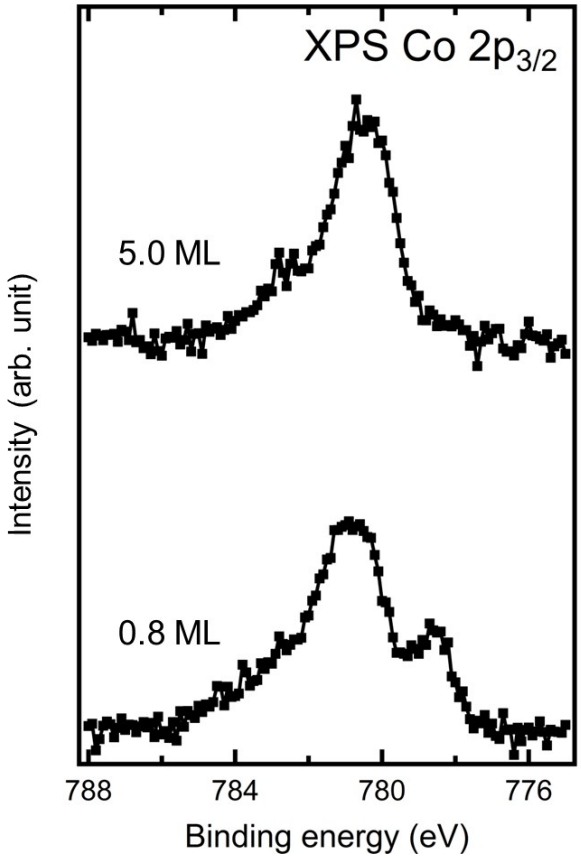

Figure S1. Al K_α Co $2p_{3/2}$ spectra of multilayer- and submonolayer CoTPP on 10 ML MgO. The observed ratio between the minority- and majority species in the monolayer is the same as for thinner MgO films (shown in the main paper).

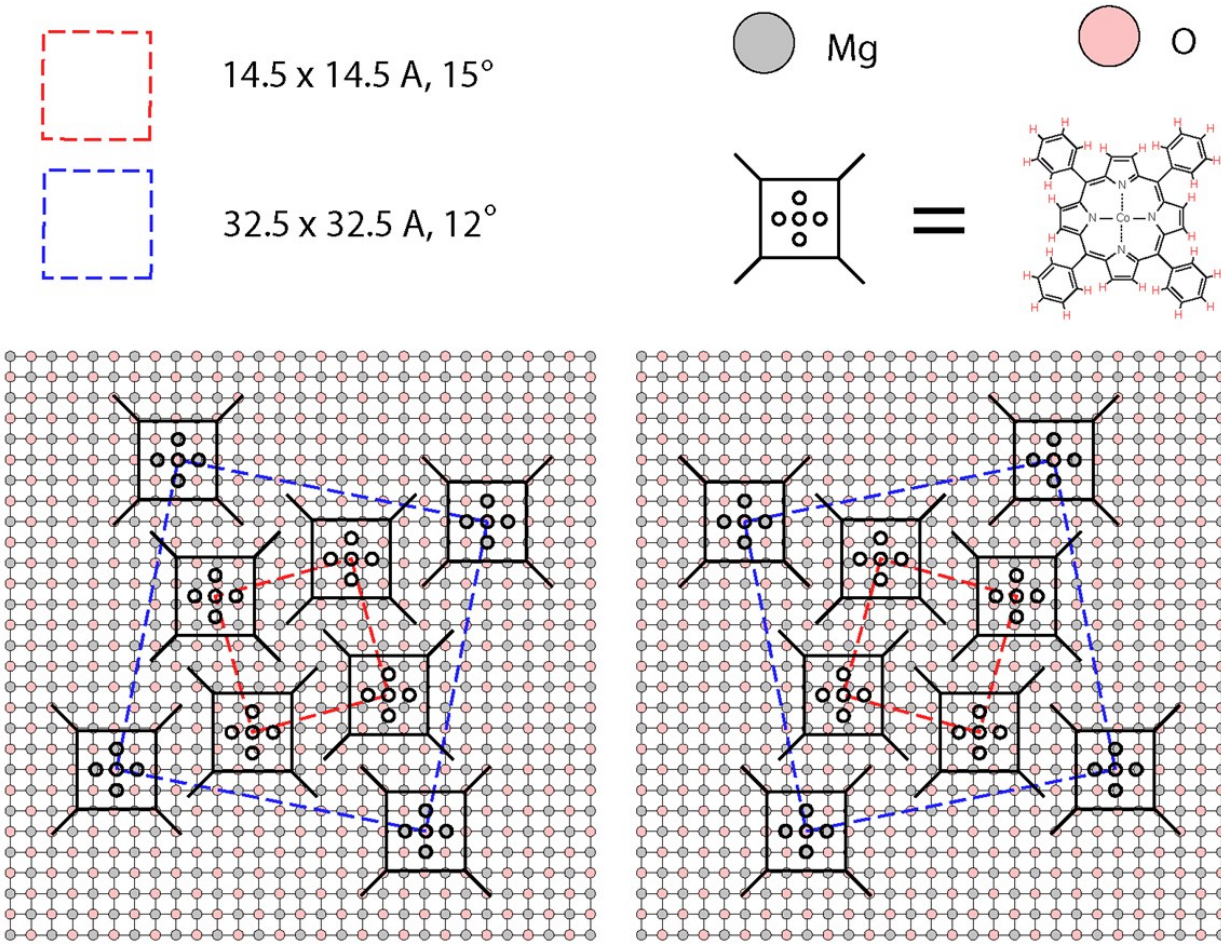

Figure S2. Structural model for a possible unit cell of CoTPP/MgO which would explain the presence of two different species in the monolayer. A square arrangement of molecules with their phenyl groups in a T-type alignment and a unit cell size of ~(14 •14) Å^2 was found in STM studies for a variety of different tetraphenylporphyrins on metal surfaces and was also therefore assumed for the structural model. If a square unit cell size of 14.5 Å^2 is chosen (red unit cell), tilted by 15° with respect to the substrate lattice, and further molecules are added, another (blue) unit cell is created. Every molecule at the corner of this larger unit cell adsorbs with its metal center directly on top of an oxygen ion. In this model, 1/5th of molecules are adsorbed on top of an oxygen ion, which would agree with the intensity ratio of the interacting to non-interacting species observed by our SR-XPS measurements. We therefore suggest that only these on-top adsorbed molecules can interact electronically with the O 2p band and create the observed new state in UPS.