**Supplementary Information**

Figs S1a and S1b show STM images of RuTPP on Cu(110). The angle and size of the STM images were calibrated using an atomically-resolved STM image of a bare Cu(110) surface, as shown in the inset of Fig. S1a. With increasing molecular coverage, the RuTPP molecule forms a regular and ordered array structure as shown in Fig. S1b.

![STM images of RuTPP adsorbed on Cu(110)](image)

The periodic DFT calculations of the geometric and electronic structure of the RuTPP and the CO-RuTPP molecules adsorbed on the Cu(110) surface were carried out using the Vienna Ab initio Simulation Package (VASP) [1]. Plane waves were used as a basis set with an energy cut-off of 400 eV. Valence electron-core interactions were included by using the projector-augmented wave method [2]. The van der Waals interactions were described using the optB86b-vdW version of the exchange-correlation functional [3-6].

The Cu surface was represented by a slab with four Cu layers. The coverage corresponds to the Aγ of CoTPP/Cu(110) structure in Ref. [7] which is the same as in the experiments. The vacuum region was 16.65 Å. Due to the large supercell, a k-point mesh of 2x2x1 was sufficient in the calculations. The short bridge adsorption site was used for the molecules. The equilibrium geometries were obtained by structural relaxations until the forces were less than 0.01 eV/Å. The two bottom layer atoms were fixed at the experimental value of 3.634 Å of the bulk lattice constant.

The local density of states was calculated in the vacuum region using the extrapolation scheme for the tails of the wave functions as described in Ref. [8].

The adsorption geometry of (CO-RuTPP/Cu(110)) was found to be very similar to the one for CoTPP/Cu(110)[7]. A top view of the structure is shown in Fig. S2. The CO molecule was found to adsorb ontop of the Ru atom in a perpendicular direction. The C-O distance was found to be 1.17 Å which is about 0.03 Å larger than the calculated distance for the isolated molecule. Upon adsorption of the molecule, the Ru–Cu distance increased by about 0.1 Å indicating a decrease in bond order between the Ru and the Cu atoms, whereas the atomic distortions of the phenyl rings increased only slightly. The DFT calculations show that the four lobed protrusions are due to the distorted phenyl groups and that the protrusion in the centre of the molecule arises from CO adsorption.

![DFT calculations of RuTPP and CO-RuTPP molecules](image)
Fig. S2 (a) Top and (b) side views of the calculated geometry of RuTPP in the $A^\gamma$ structure on Cu(110). (c) Top and (d) side views of the calculated geometry of CO-RuTPP in the $A^\gamma$ structure on Cu(110).

Fig. S3 (a) (b) Simulated, topographical STM images of (a) RuTPP and (b) CO-RuTPP in the $A^\gamma$ structure on Cu(110). The sample biases are (a) 0.5 V and (b) 1.0 V. The average heights are (a) 10.7 Å and (b) 10.8 Å from the outermost Cu surface plane. (c) STM image of RuTPP and CO-RuTPP on Cu(110) as already shown in Fig. 3(a) in the main text.
Fig. S4 Calculated local density of states (LDOS) at 9.15 Å above the Cu surface layer at the centre of RuTPP/Cu(100) and CO-RuTPP/Cu(110).

References