Supporting Information

Octaethyl *vs.* Tetrabenzo Functionalized Ru Porphyrins on Ag(111): Molecular Conformation, Self-Assembly and Electronic Structure

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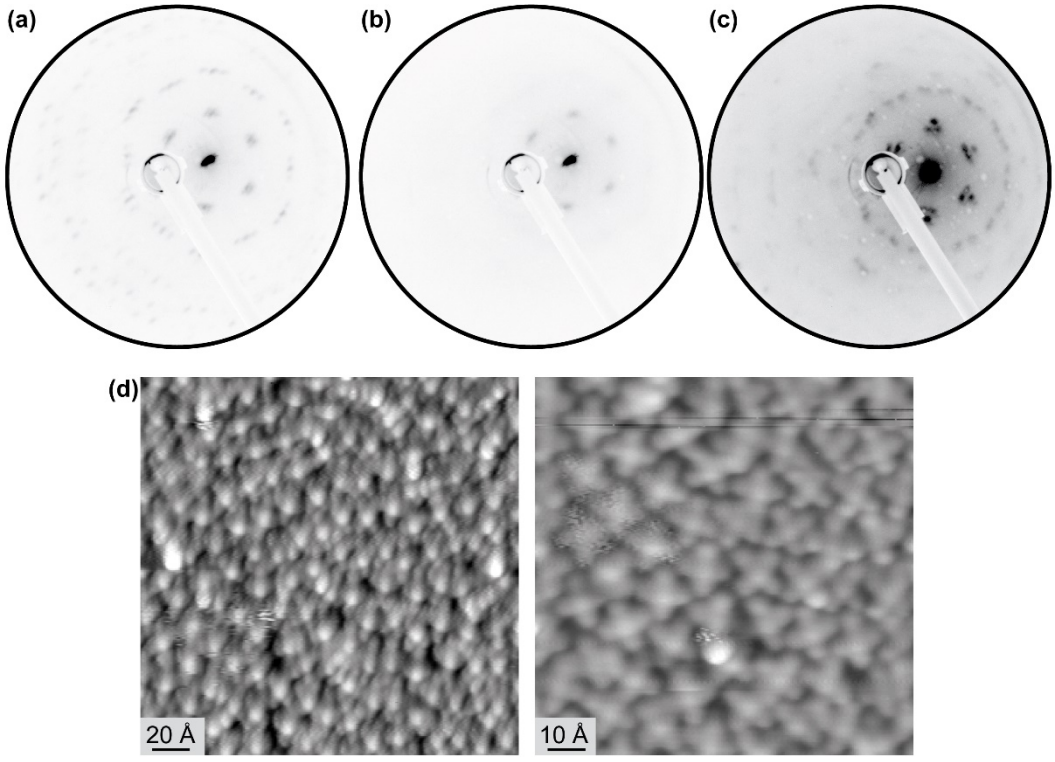

Figure S1. LEED of (a) compressed phase of Ru-OEP, (b) after annealing to 600 K, and (c) Ru-TBP prepared on a sample at 700 K. All LEED patterns were taken with an electron energy of 30 eV. (d) STM images of a monolayer of Ru-OEP annealed to approximately 600 K (left: -1768 mV, 80 pA, RT; right: 1768 mV, 110 pA, RT).

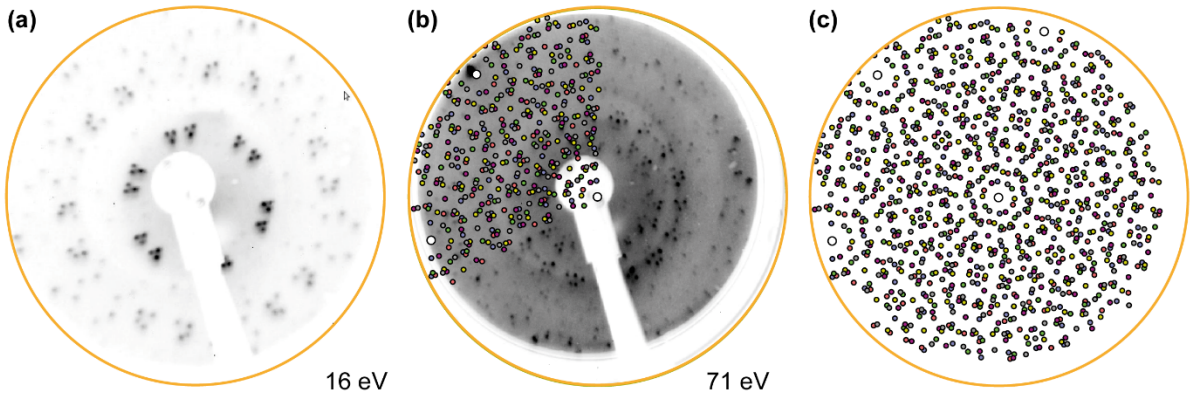

Figure S2. (a-b) LEED of relaxed phase Ru-OEP on Ag(111). On the top left of (b) the simulated pattern is overlayed for comparison. The respective electron energy is noted at the bottom right of the image. (c) Complete simulated pattern.

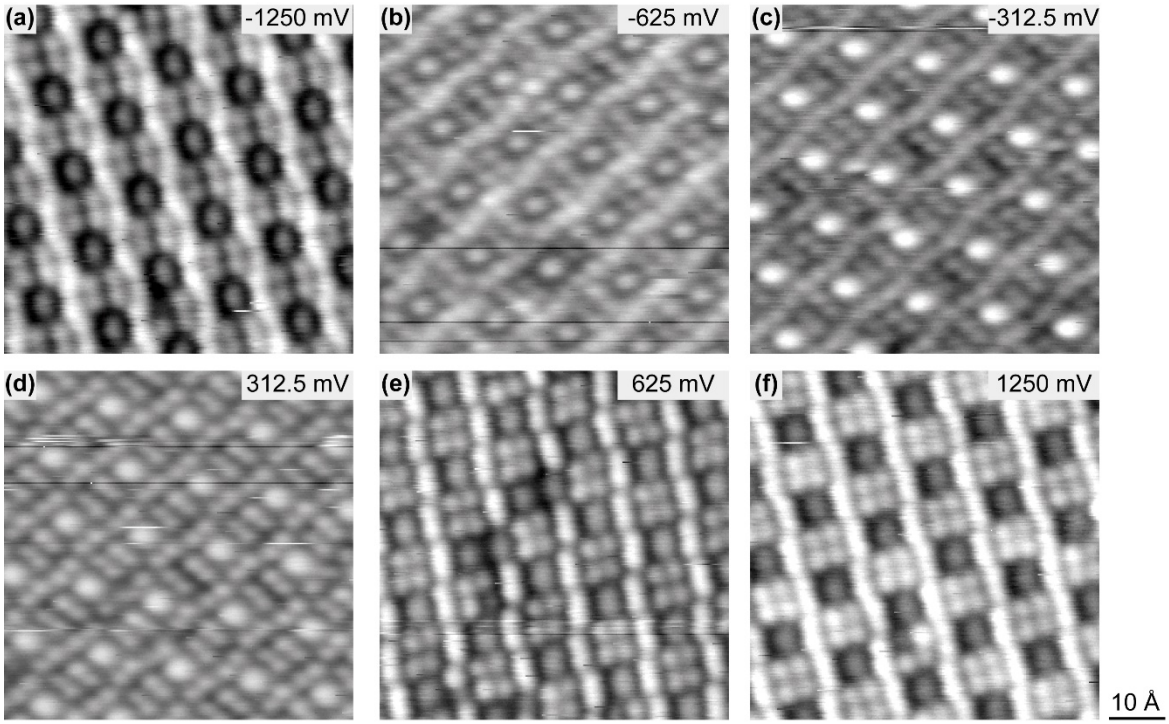

Figure S3. STM images of compressed phase of Ru-OEP on Ag(111) at different biases at rt (a: 30 pA; b: 20 pA; c: 20 pA; d: 50 pA; e: 60 pA; f: 40 pA). The positive and negative bias at 1250 mV shows a darker porphyrin center compared to the ethyl side chains. This is well matching with the valence band measurements, which show a state at 0.51 eV and no state at 1.25 eV beneath Fermi.

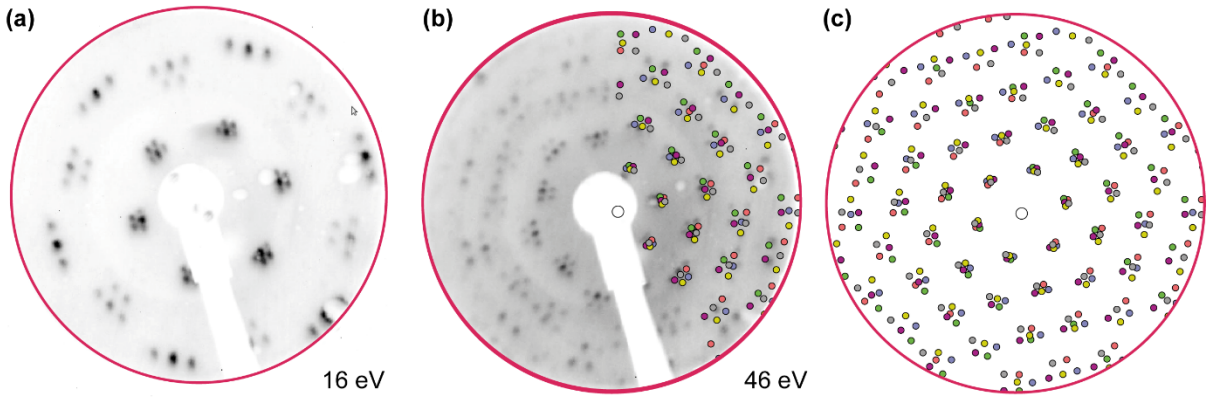

Figure S4. (a-b) LEED of the compressed phase Ru-OEP on Ag(111). On the top left of (b) the simulated pattern is overlayed for comparison. The respective electron energy is noted at the bottom right of the image. (c) Complete simulated pattern.

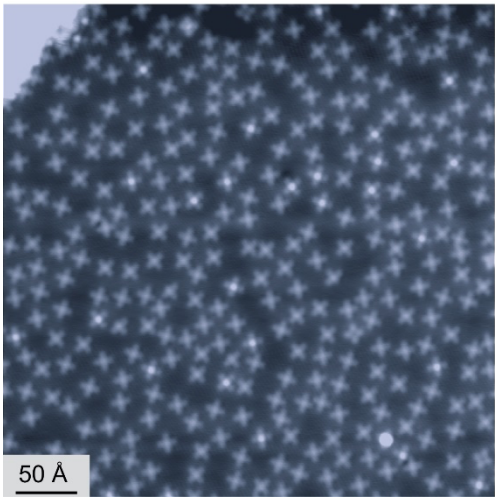

Figure S5. STM image of low coverage Ru-TBP on Ag(111) (50 pA, 200 mV, 6 K).

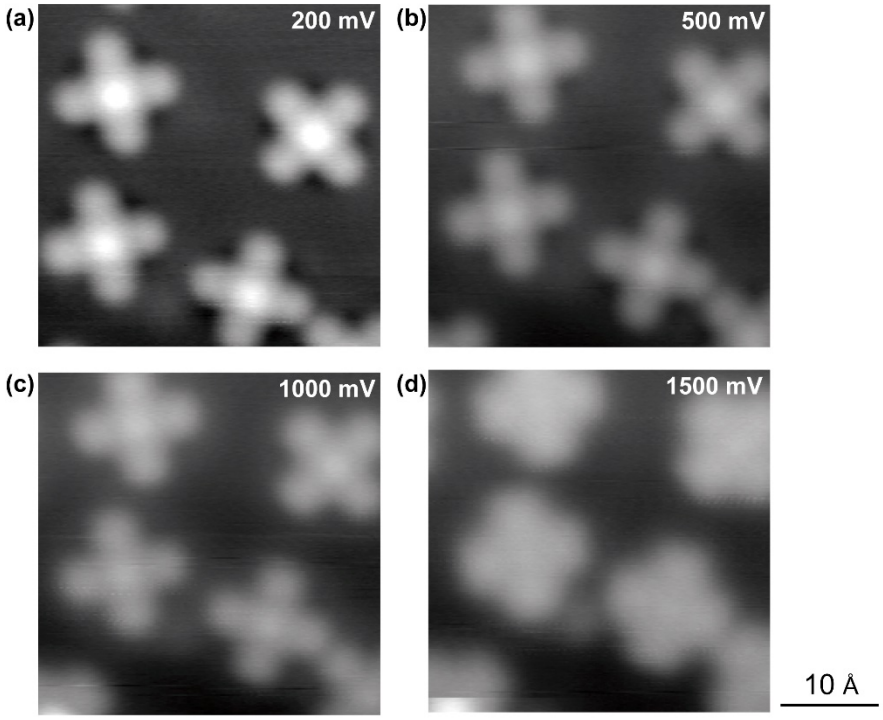

Figure S6. (a-d) STM images of Ru-TBP on Ag(111) at 5 K, captured at different biases as indicated in each image. All images were acquired at 20 pA.

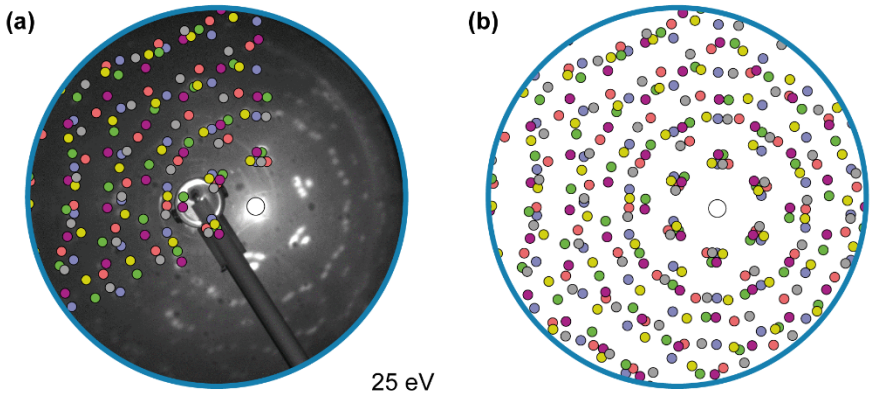

Figure S7. (a) LEED of Ru-TBP on Ag(111). On the top left the simulated pattern is overlayed for comparison. The respective electron energy is noted at the bottom right of the image. (c) Complete simulated pattern.

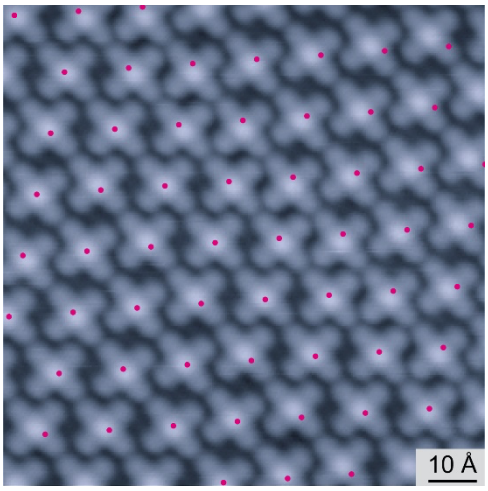

Figure S8: Position of Ru-TBP derived by LEED at 200 K (pink dots) overlaid over an STM image (50 pA, 200 mV, 5 K). Small deviations between the LEED positions and the STM image are observed. This is ascribed tentatively to the different acquisition temperature of the techniques.

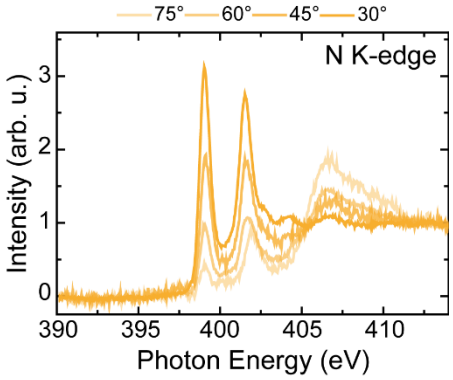

Figure S9. N K-edge NEXAFS measurements of the relaxed phase of Ru-OEP on Ag(111) acquired at four different incidence angles. The spectra exhibit a pronounced dichroism in the π* region comparable to the compressed phase of Ru-OEP on Ag(111).