Chemical Communications

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Electronic Supplementary Information

for

Following the steps of a reaction by direct imaging of many individual molecules

Dennis van Vörden,[a] Ben Wortmann,[a] Nico Schmidt,[a] Manfred Lange,[a] Roberto Robles,[b] Lothar Brendel,[a] Christian A. Bobisch[a] and Rolf Möller[a]

[a] University of Duisburg-Essen, Faculty of Physics, Center for Nanointegration Duisburg-Essen, Lotharstrasse 1-21, 47057 Duisburg, Germany. Fax: +49-203-379-1727; Tel:+49-203-379-4220; E-mail: christian.bobisch@uni-due.de, rolf.moeller@uni-due.de

[b] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain.

All experiments as well as the sample preparation are performed in an ultrahigh vacuum system. The Cu(111) surface is prepared by several cycles of sputtering by Ar^+ ions at a kinetic energy of 2.5 keV (45 min at ≈15 μA/cm^2) and annealing to 880 K for 90 min. The preparation is checked by low energy electron diffraction (LEED). The 2,3,7,8,12,13,17,18-octaethylporphyrin Fe(III) chloride (FeOEP-Cl) used in our experiments has a purity of 98% according to the retailer Porphyrin Systems. The molecules are thermally evaporated from a tiny oven with a quartz crucible heated by a tungsten filament to a temperature of 500 K. Prior to the experiments, the oven was carefully outgassed. The flow of molecules is checked by a quadrupole mass spectrometer (QMS) covering the range from 1 to 1028 amu. Three QMS spectra with different electron energies used to ionize the molecules are presented in Fig. S 1. With increasing ionization energy, the number of dechlorinated molecules in the QMS rises. Therefore, only a lower limit of at least 60% chlorinated molecules out of all sublimated molecules can be given. More information about the ratio of chlorinated to dechlorinated molecules after adsorption can be found in an earlier publication.[1] Here a submonolayer is deposited onto the copper surface at room temperature. Previous experiments showed that depending on the sample temperature during preparation two different species - chlorinated and dechlorinated species - are observed. Beside these, no further species or fragments are found on the surface.

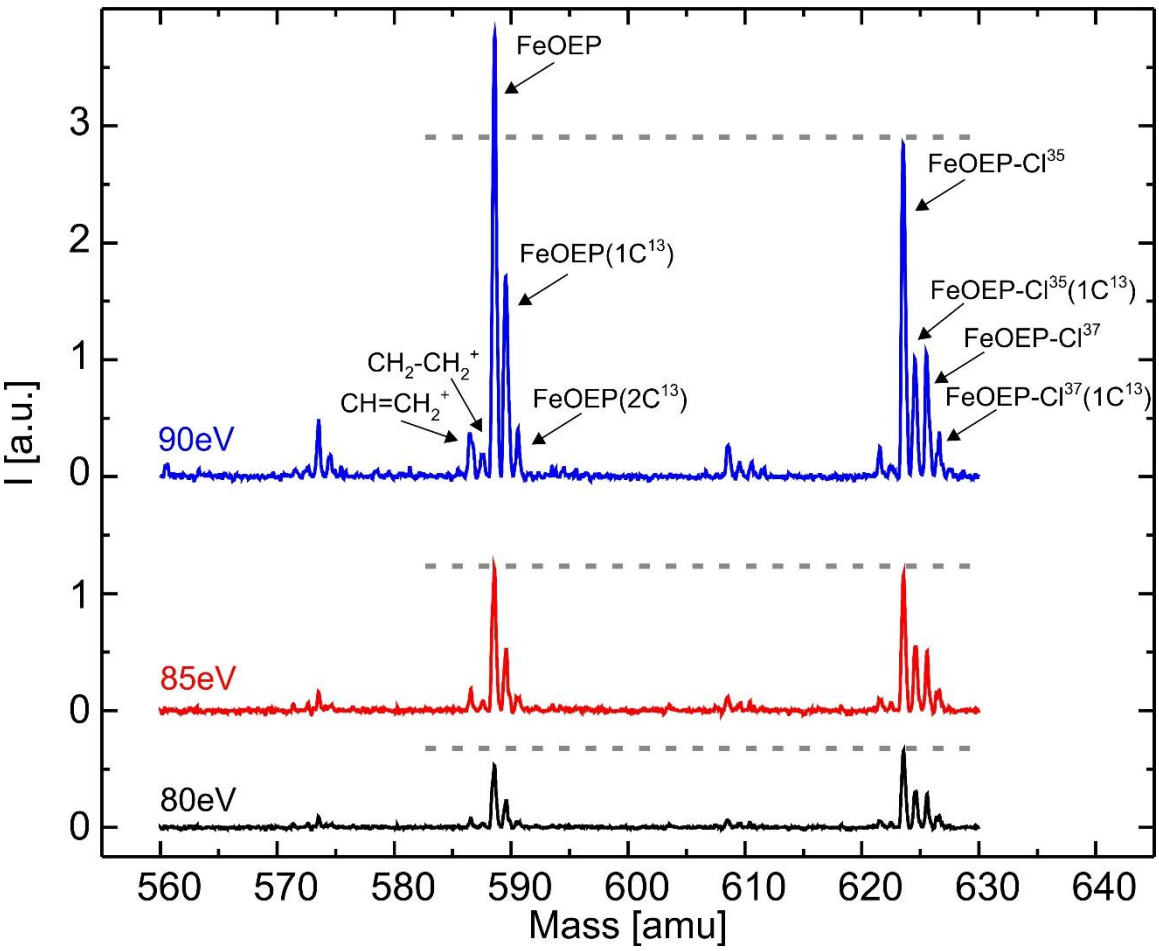

Fig. S 1: QMS data of FeOEP and FeOEP-Cl for different electron energies used for ionization.

The STM images are obtained using a home-built low-temperature scanning tunneling microscope (STM) in ultra-high vacuum at T = 80 K. The tunneling tips are electrochemically etched from a tungsten wire with a diameter of 100 µm. They are further prepared in situ by field emission in front of a Au(111) surface. The data are acquired using the GxSM[2] software and further processed by the WSxM[3] software.

[1]D. van Vörden, M. Lange, J. Schaffert, M. C. Cottin, M. Schmuck, R. Robles, H. Wende, C. A. Bobisch and R. Möller, *ChemPhysChem*, 2013, 14, 3472–3475.
[2]P. Zahl, Th. Wagner, R. Möller, A. Klust, J. Vac. Sci. Technol. B 28, C4E39 (2010)
[3]I. Horcas, R. Fernandez, J.M. Gomez-Rodriquez, J. Gomez-Herrero and A.M. Baro, Rev. Sci. Instrum. 78, 013705 (2007)