

Supporting Information

Oxidation of an organic adlayer - a bird's eye view

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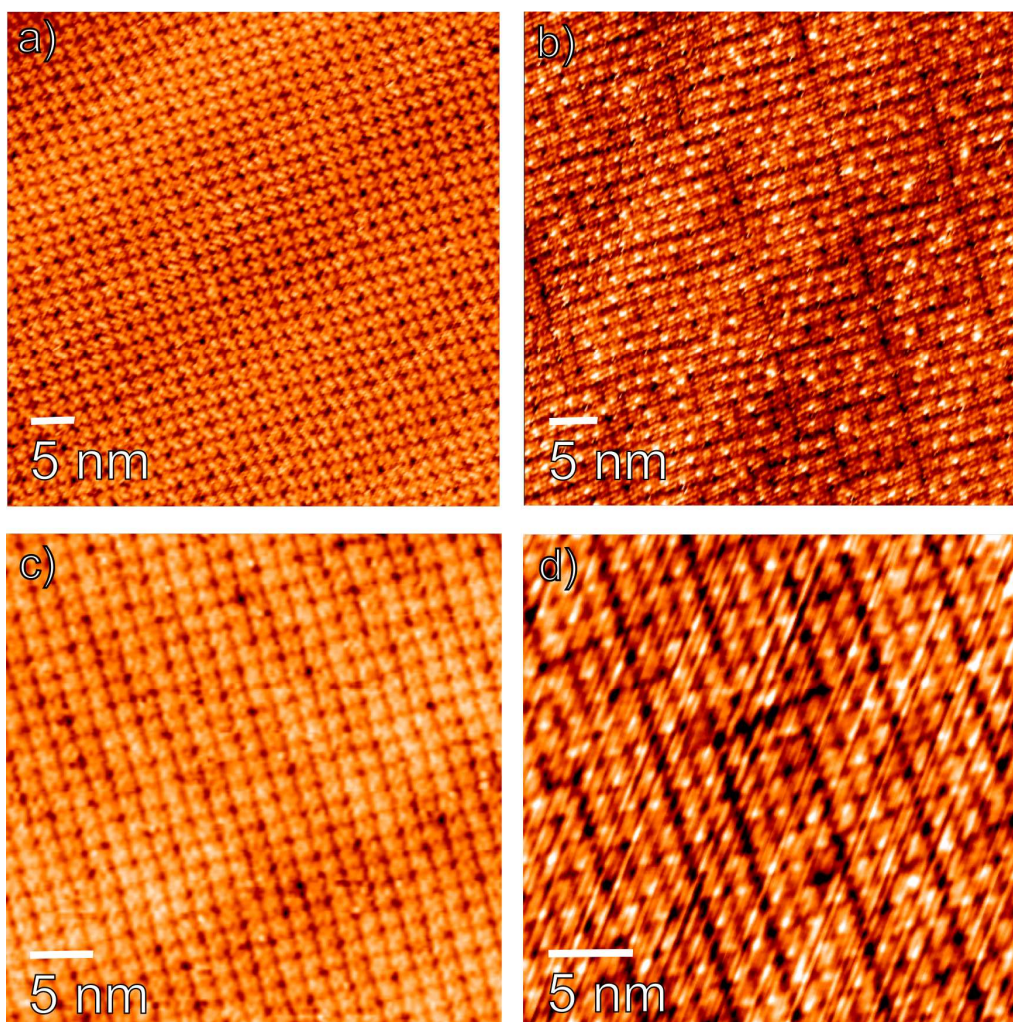


Figure S1 Large scale STM images

- a) α - phase on Ag(111) ($48 \times 48 \text{ nm}^2$, 154 s frame^{-1} , $I_T = 60 \text{ pA}$, $U_T = -2.29 \text{ V}$)
- b) α' -phase on Ag(111) ($45 \times 45 \text{ nm}^2$, 176 s frame^{-1} , $I_T = 70 \text{ pA}$, $U_T = -1.96 \text{ V}$)
- c) α -phase on Ag films ($36 \times 36 \text{ nm}^2$, 100 s frame^{-1} , $I_T = 5 \text{ pA}$, $U_T = -2.20 \text{ V}$)
- d) α' -phase on Ag films ($28 \times 28 \text{ nm}^2$, 100 s frame^{-1} , $I_T = 15.8 \text{ pA}$, $U_T = -2.25 \text{ V}$).

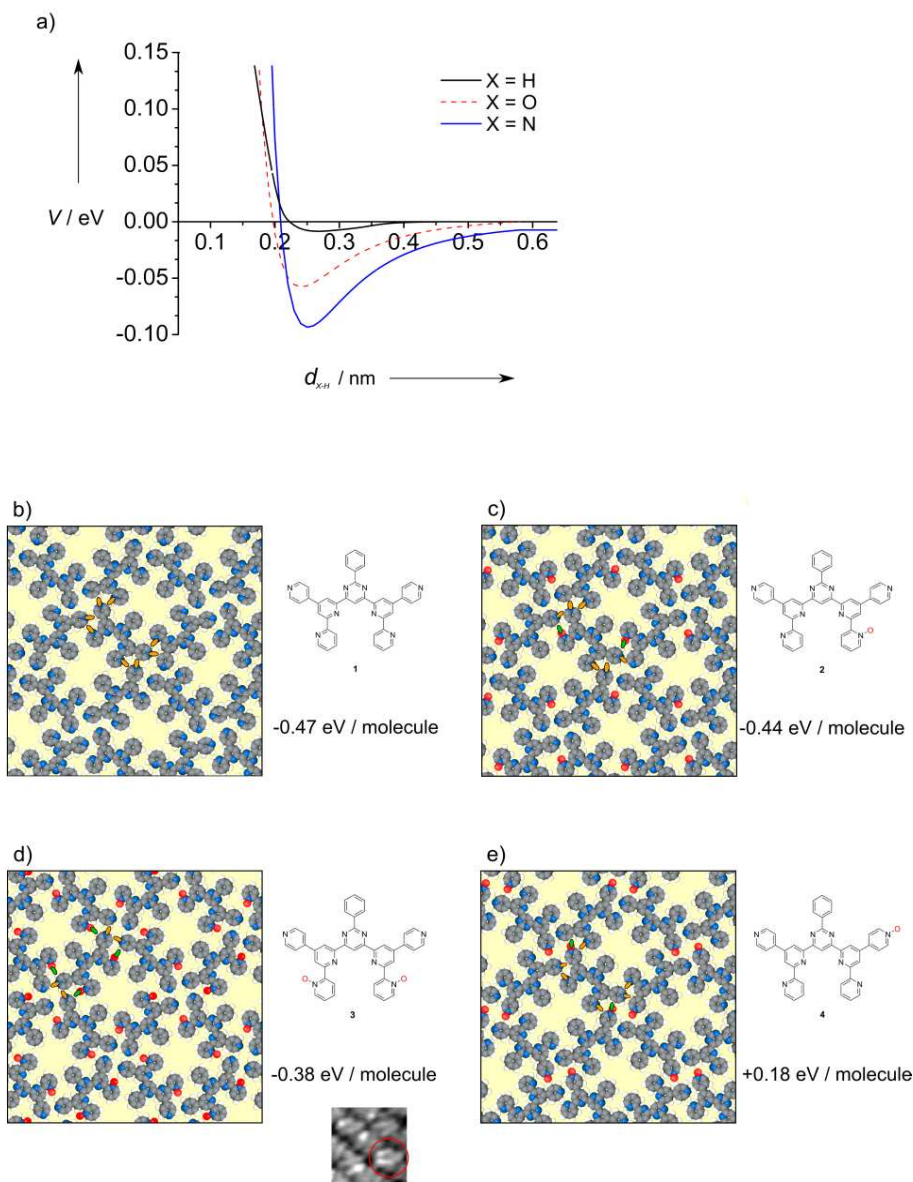


Figure S2

a) MP2 (6-31G(d,p)) based $O\cdots H$ (calculated in this work), $N\cdots H-C^{15}$ and $C-H\cdots H-C^{15}$ potentials used in the MC based structure relaxations. (b) - (e): Relaxed structures of the periodic MC based calculations. Hydrogen bonds are marked for one molecule per structure (C: grey, N: blue, O: red, $N\cdots H$ bonds: orange, $N-O\cdots H$ bonds: green). b) α -phase (model for the structure in Figure 1a). c) Network of **2** (model for the structure in Figure 1b). d) Network of **3** (rarely observed). The inset shows an STM image of one **3** molecule ($4.5 \times 4.5 \text{ nm}^2$, 1 frame s^{-1} , $I_T = 50.1 \text{ pA}$, $U_T = -1.75 \text{ V}$). e) Network of **4** (not

observed).

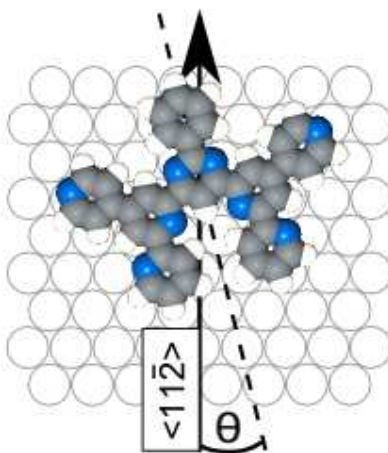


Figure S3

Definition of the azimuth angle θ of **1** with respect to the $\langle 11\bar{2} \rangle$ direction of Ag(111) and Au(111).