# Supporting information for: Study of Ferrocene Dicarboxylic Acid on Substrates of Varying Chemical Activity

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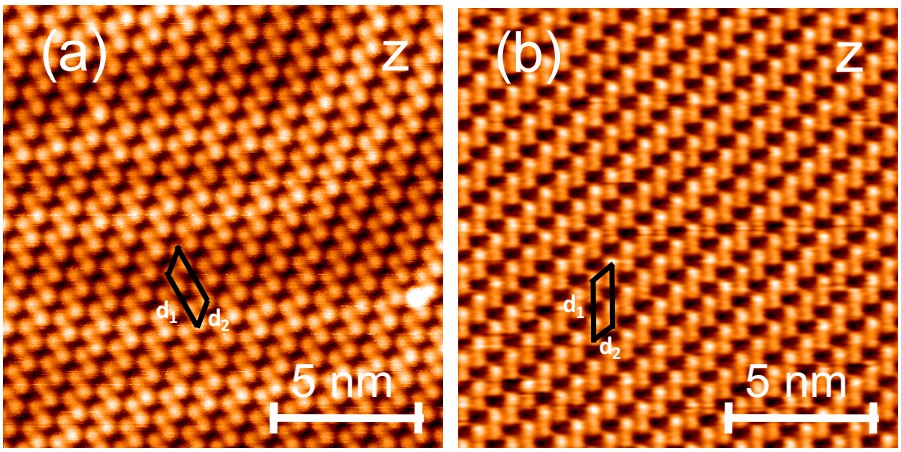


Figure S1: STM topography images of detail of self assembled molecular islands of FcDA molecules on Au(111) (a) and Ag(111) (b). In both cases a molecules were evaporated for 2 minutes at T = 145°C on to sample hold at room temperature. From direct comparison of FcDA on Au(111) and Ag(111) is visible, that one can expect similar behaviour on both substrates. a) STM topography image of self assembled FcDA molecule on Au(111). Images is taken at room temperature, U = 1.5 V, $I_t$ = 50 pA, size is 15×15 nm$^2$. There is visible typical herringbone structure of clean Au(111). Black rhomboid represents unit cell, with dimensions: $d_1$ = 2.1 nm and $d_2$ = 0.8 nm. b) STM topography image of self assembled FcDA molecule on Ag(111). Black rhomboid represents unit cell, with dimensions: $d_1$ = 2.2 nm and $d_2$ = 0.9 nm. Images is taken at T ∼ 1.2 K, $U$ = 100 mV, $I_t$ = 15 pA, size is 15×15 nm$^2$.

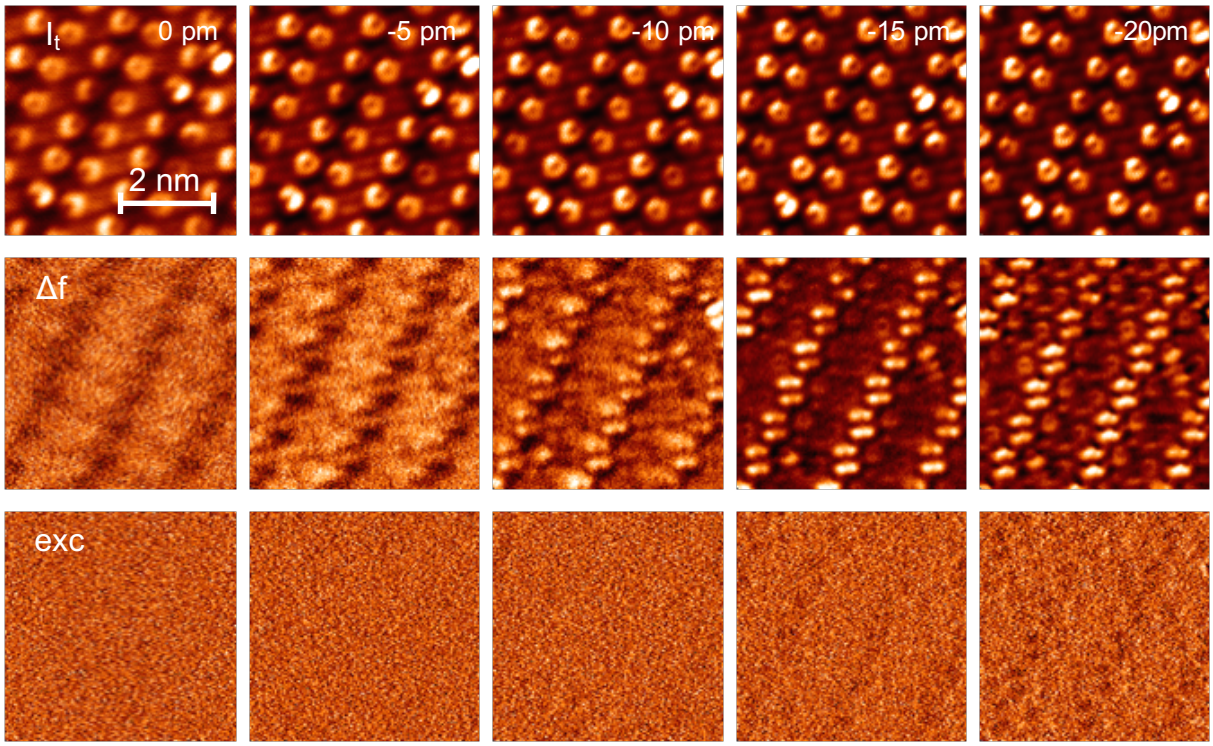


Figure S2: Successive constant height images of the simultaneously acquired of tunneling current (top row), frequency shift (middle row) and excitation (bottom row) of FcDA reconstruction on Ag(111) taken with CO decorated tip. Each column of images is taken at a tip height 5 pm closer to surface than the previous, starting from the first column on the left. You can see typical double line pentagonal feathers in STM. These pentagons are referred to FcDA molecule with rings parallel to the substrate. Typical double lobe feature, molecules in the position of ring perpendicular to the substrate, is seen on frequency shift. There is some contrast in excitation channel when you are getting close to the sample. In this case, contrast is visible from column labeled as -15 pm. Imaging parameters: 5×5 $nm^2$, -10 mV.

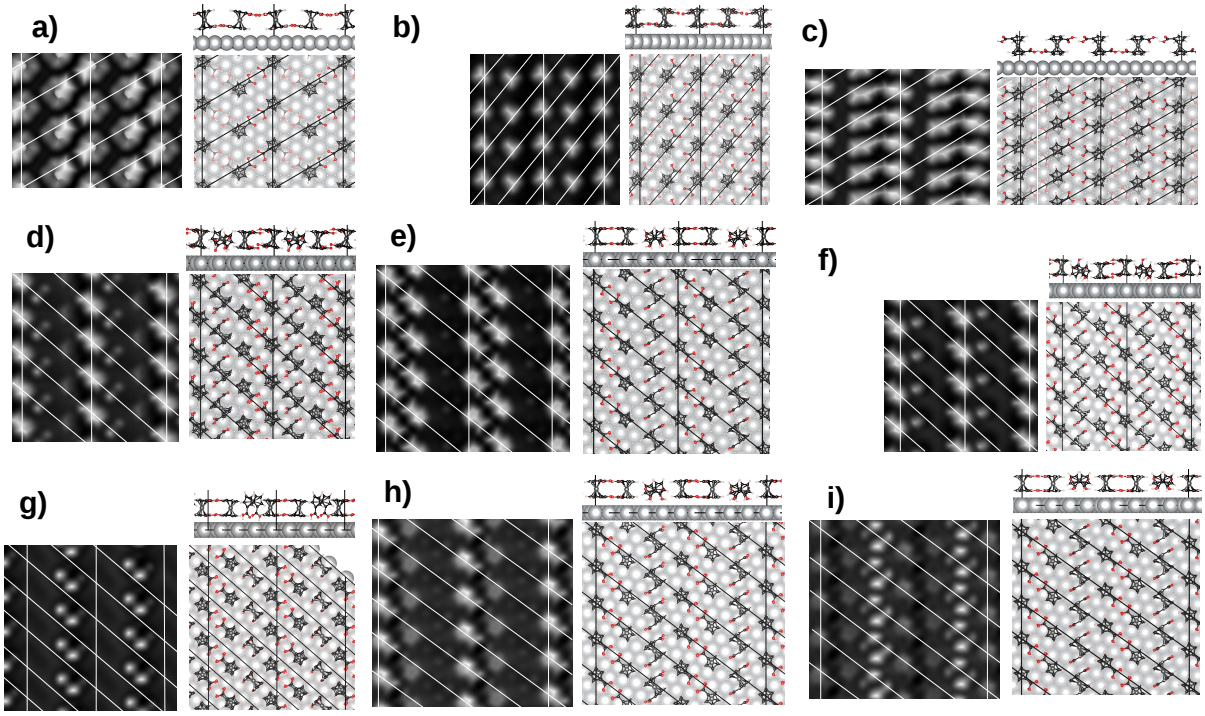


Figure S3: Geometrical models of selected periodic structures of FcAD molecules at the Ag(111) substrate together with simulations of their ncAFM images. The structures a)-h) was obtained by a full geometry relaxation using DFT method. The structure i) is derivated from the structure h) by moving each of the FcAD monomers by 0.8 Å outward the substrate. Prameters of ncAFM dimulations: CO probe-particle ($q = -0.1e$), $k_{xy} = 0.5$ N/m.

Table S1: Average binding energies $< E_b >$ of FcAD molecules at the Ag(111) substrate forming different adsorption structures (see Figure **??**). All values in eV.

| a) | b) | c) | d) | e) | f) | g) | h) |
|---|---|---|---|---|---|---|---|
| -2.52 | -2.52 | -2.52 | -2.45 | -2.61 | -2.38 | -2.52 | **-2.61** |

$$< E_b >= \frac{1}{N} \left( E_{tot} - N \cdot E_{mol} - E_{sub} \right), \tag{1}$$

$E_b$ - molecule binding energy, $E_{tot}$ - energy of the whole adsorption system, $E_{mol}$ - energy of free-standing molecule, $E_{sub}$ - energy of substarte, $N$ number of molecules in a super-cell.

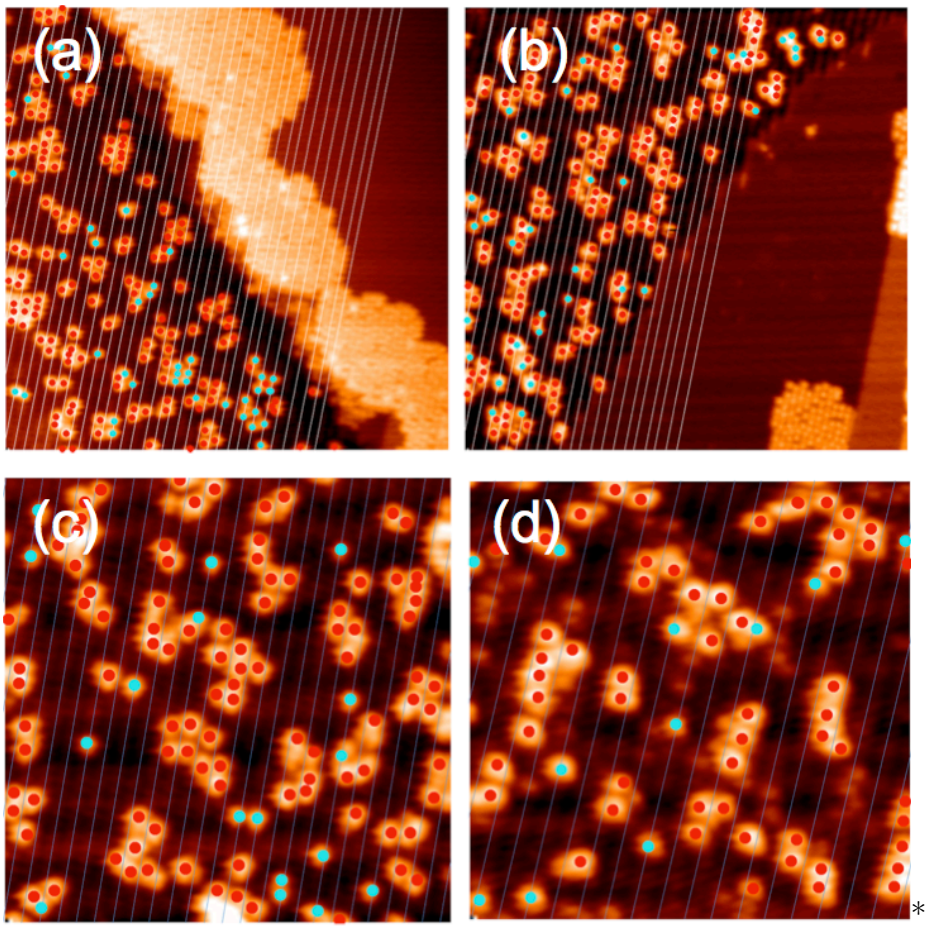


Figure S4: Overview images on different $Cu_3N/Cu(110)$ with FcDA molecules. White lines are enhancing position of nitrogen rows of $Cu_3N/Cu(110)$. Red dots represent moleculeabsorb on valley position, cyan dots correspond to on row position, In all figures. Figures are taken in constant current mode with bias voltage U = 0.5 V, current setpoint I = 0.2 nA, with different metallic tips (a) There are146 FcDA molecules (78.9% ± 6.5% are in valley position) , (b) There are144 FcDA molecules (82.6% ± 6.9% are in valley position), (c) There are 97 FcDA molecules (85.1% ± 8.6% are in valley position), (d) There are 55 FcDA molecules (83.3% ± 11.2% are in valley position).

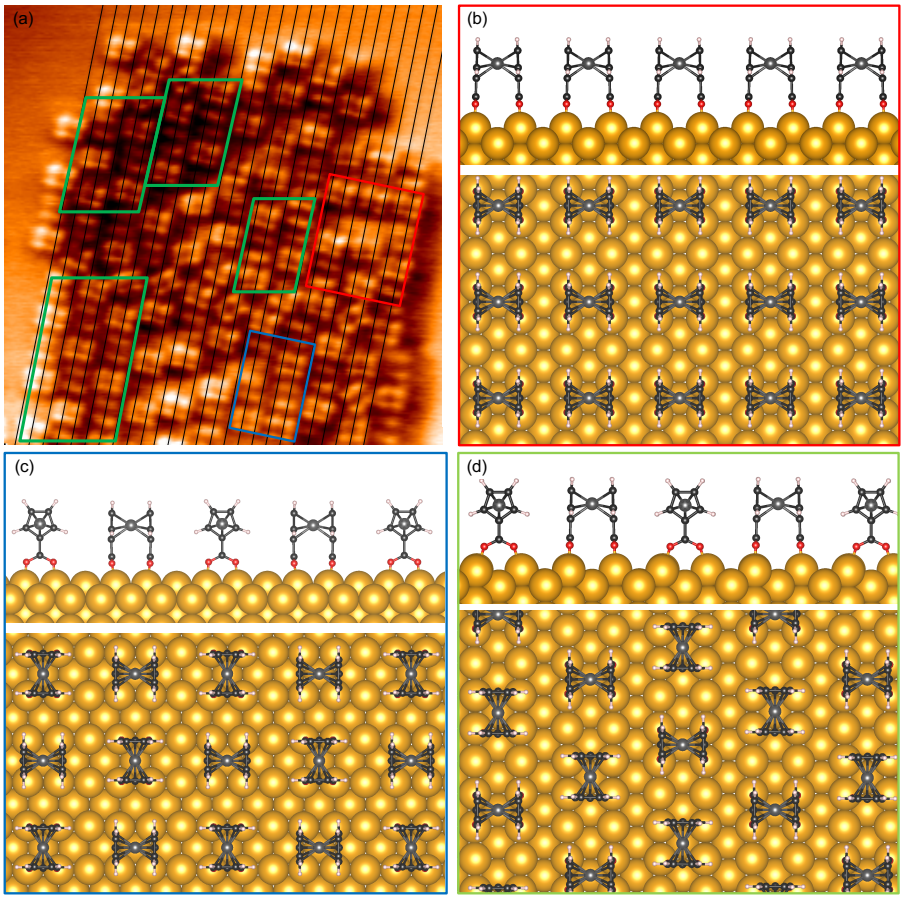


Figure S5: Island of self-assembled FcDA molecules deposited on Cu(110) visualized in frequency shift channel at constant height. Image is overlaid by parallel black lines that corresponds to the positions of Cu rows of Cu(110). We obtained a correct direction of Cu rows by extrapolating position of nitrogen rows in $Cu_3N$/Cu(110) island occupying the same terrace. Green rhomboids denote FcDA molecules reconstruction introduced in main text. Blue rectangle highlights area with orthogonal ordering of FcDA molecules. Calculated model for orthogonal ordering is blue frame. Red rectangle marks next possible order of FcDA molecules in the island. Size of frequency shift image is $10 \times 10$ $nm^2$, U = 10 mV.

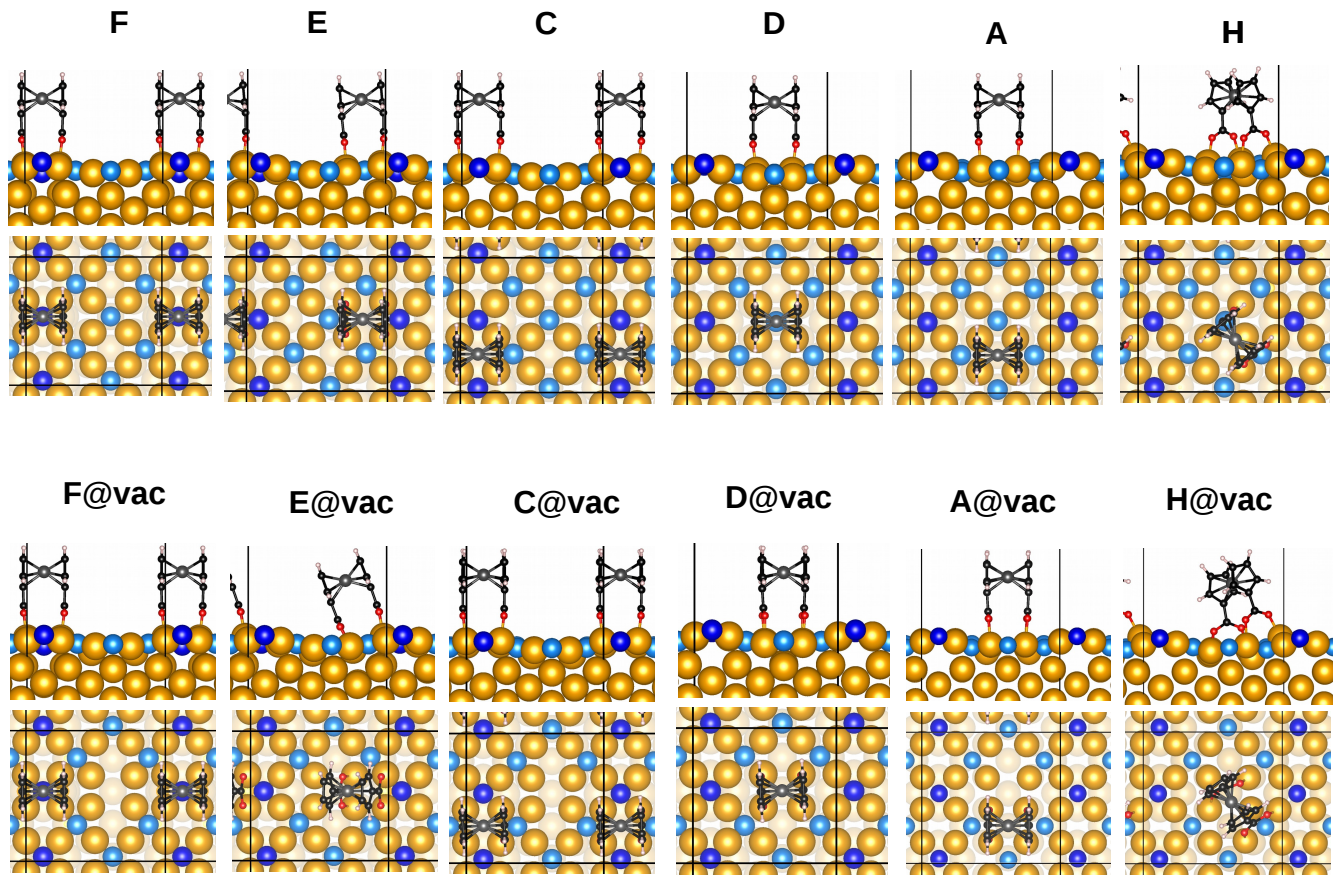


Figure S6: Energetically stable configurations of the dehydrogenated FcDA molecules at different adsorption sites of $Cu_3N/Cu(110)$ substrate (stoichiometric and vacanced) simulated with DFT method. For binding energies see Table **??**.

Table S2: Binding energies $E_b$ of the dehydrogenated FcDA molecules at different adsoprtion sites (see Figure **??**) of $Cu_3N/Cu(110)$ substrate caluclated with DFT method. All values in eV.

| | F | E | C | D | A | H |
|---|---|---|---|---|---|---|
| @clean | -3.56 | -3.31 | -3.12 | -3.03 | -2.98 | -2.54 |
| @vac | -3.19 | -3.49 | -2.92 | -3.73 | -2.83 | **-3.79** |

$$E_b = E_{tot} - E_{mol} - E_{sub} \tag{2}$$