Supporting Information: Assembly of Ferrocene Molecules on Metal Surfaces Revisited

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Supporting Information

Figure S1 shows STM images acquired after deposition of ferrocene on Cu(100). In the large scale image of Figure S1(a) we see how for a ferrocene coverage below the monolayer, Cu(100) areas remain clean in between long-range ordered molecular layers. In Figure S1(b-d) we can distinguish the presence of the same compact and zigzag assemblies as on Cu(111). Table S1 presents the unit cell parameters for both arrangements as well as the apparent height of the molecular layer, which are almost identical to the parameters obtained for Cu(111). The fact that the substrate orientation does not influence the adsorption configuration of ferrocene suggests that the molecules have a weak coupling with the substrate, meaning that they are physisorbed. The low associative desorption temperature observed for this system, around 200 K, also supports the idea of a feeble substrate-molecule coupling. Reinforcing this idea we find that the rotational domains observed for each configuration in the Cu(111) surface, (0°, 30°, 60°) for the compact and (17°, 50°) for the zigzag, are also observed in Cu(100). This implies that the rotational domains are only related to the symmetry of the molecular layer itself and not to the one of the substrates.

Table S1: Apparent height of the molecular layer with respect to Cu(100) ($\mathbf{h}_{Cu-FeCp_2}$) and unit cell parameters ($\mathbf{a'_1}$, $\mathbf{a'_2}$, $\mathbf{b'_1}$, $\mathbf{b'_2}$, θ) of both compact and zigzag arrangements.

	$\mathbf{h}_{Cu-FeCp_2}$(Å)	$\mathbf{a'_1}$ (Å)	$\mathbf{a'_2}$ (Å)	θ (°)
Compact	3.1±0.1	9.0±0.3	16.0±0.3	90±3

	$\mathbf{h}_{Cu-FeCp_2}$ (Å)	$\mathbf{b'_1}$ (Å)	$\mathbf{b'_2}$ (Å)	θ (°)
Zigzag	3.1±0.1	23.0±0.4	13.0±0.4	72±3

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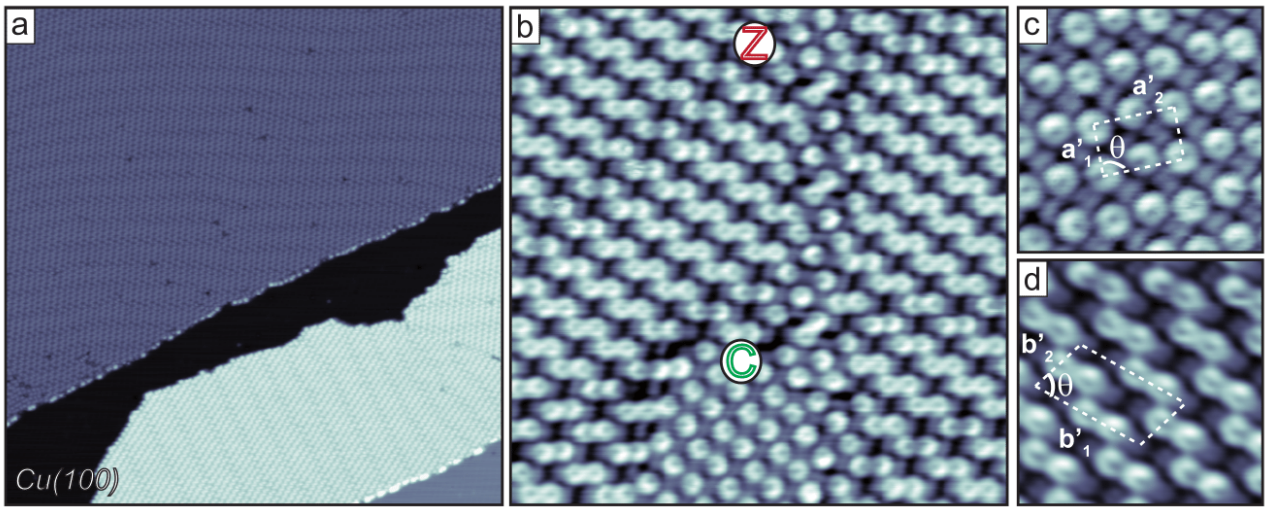

Figure S1: Ferrocene adsorption on Cu(100): (a) Bare Cu(100) areas are observed in between well ordered ferrocene monolayers, (b) Both compact (C) and zigzag (Z) arrangements appear on the surface, (c-d) A zoom and the unit cells marked in white of both configurations, compact and zigzag respectively, are shown. Image parameters: (a) (-1 V, 0.2 nA), (b) (0.5 V, 1 nA), (c) (-1 V, 1 nA), (d) (0.15 V, 1 nA). Image sizes: (a) $100 \times 100\text{nm}^2$, (b) $15 \times 15\text{nm}^2$, (c-d) $5 \times 5\text{nm}^2$.