DFT study of the Moiré Pattern of FeO monolayer on Au(111)

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1. Supporting Information

To check if a fourth layer of Au would change the picture we optimized the geometry of the fcc small model with four layers of gold. The properties of the interface do not change with respect to the three layers case, as shown in Table S1. We also added a fourth layer of gold to the moiré structure and run a single point calculation. Simulated STM images at both negative and positive biases keep the same contrast seen for the three layer case (see Figure S1), assuring that the electronic density of states around the Fermi level is not modified adding a fourth layer of Au. Given these evidences we believe that considering three layer of Au we are able to accurately describe the FeO/Au interface keeping the calculations under manageable computational conditions, also considering the large dimension of the moiré cell.

Table S1: Properties of the fcc high-symmetry domain, here modelled as (2x2) cell with a lattice parameter of 3.06 Å with 3 and 4 layers of Au substrate. l is lattice parameter (Fe-Fe distance), Δz_{Fe-O} is the rumpling (computed as $z_O - z_{Fe}$), Δz_{FeO-Au} is the interface distance (height difference between FeO and the first layer Au, computed as $(z_{Fe} + z_O/2 - z_{Au})$, d_{Fe-O} is the Fe-O distance, $q_{Fe,O}$ is the Bader charge and μ_{Fe} is the iron magnetic moment. Adhesion energy (E_{ad}) and interface charge transfer towards the substrate (CT) are given per FeO unit. $\Delta\Phi$ is the difference between the work function of the FeO/Au system and of the bare Au(111) surface, reported in brackets.

structure	l[Å]	Δz_{Fe-O}[Å]	Δz_{FeO-Au}[Å]	d_{Fe-O}[Å]	q_{Fe}[e]	q_O[e]	$\mu_{Fe}[\mu_B]$	E_{ad}	CT	$\Delta\Phi$ [eV]
fcc 3 Au	3.06	0.68	2.48	1.87	+1.31	-1.03	±3.71	-0.66	-0.28	+0.31(+5.44)
fcc 4 Au	3.06	0.68	2.49	1.88	+1.51	-1.20	±3.72	-0.65	-0.30	+0.32(+5.43)

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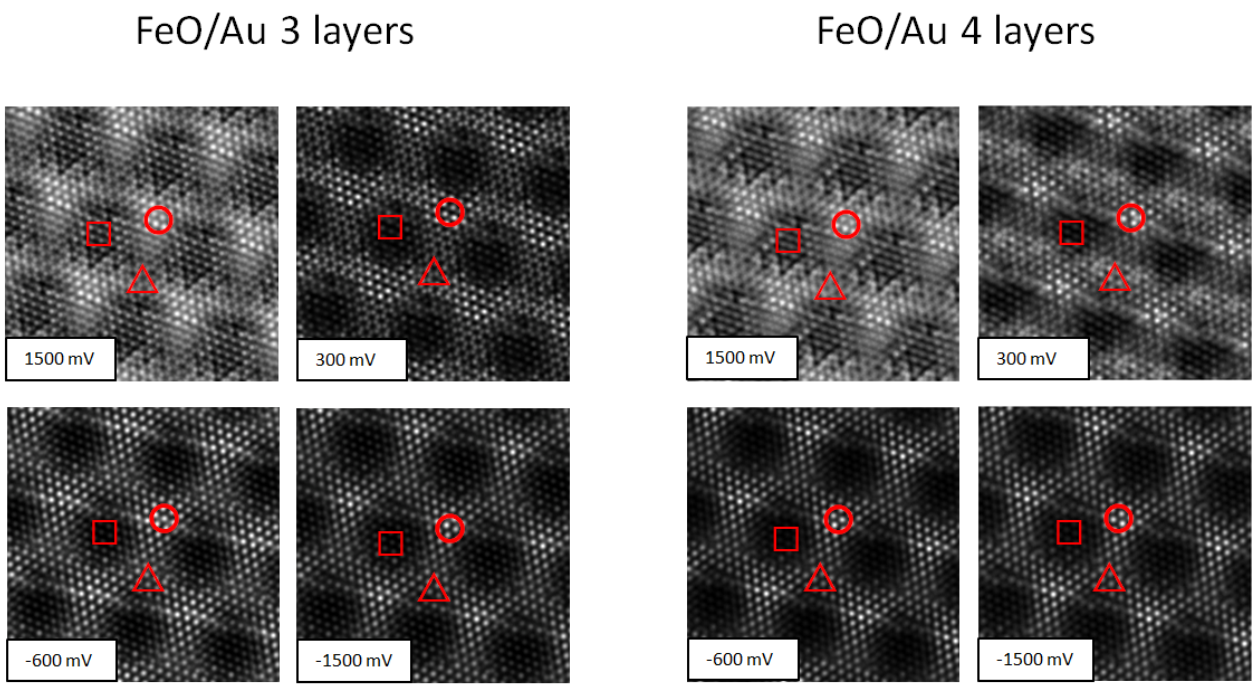

Figure S1: STM images for the FeO/Au moiré superstructure computed at different biases. Left: 3 layers of Au substrate, right: 4 layers of Au substrate considered in the calculation. Symbols mark the three high-symmetry domains: □ fcc, △ hcp, and ○ top. Computed images are taken at 2.5 Å above the FeO layer.