Supporting information for

Calculated and structural analysis of self-assembly formed by [7]thiaheterohelicene-2,13-carboxaldehyde molecules on Au(111)

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Computational methods

In order to predict adsorption geometries of molecules on a surface, we have performed calculations based on the atom-superposition and electron-delocalization molecular-orbital method.

Computational details

Calculations were performed by using numerical methods based on Hückel molecular orbital theory. Atomic orbitals parameters are given in the following table with ionization potential (IP) in eV and Slater orbital exponents (ξ) in au.

atom	orbital	IP (eV)	ξ_1	c_1	ξ_2	c_2
C	2s	−21.4	1.625	1.0		
	2p	−11.4	1.625	1.0		
H	1s	−13.6	1.300	1.0		
O	2s	−32.3	2.275	1.0		
	2p	−14.8	2.275	1.0		
S	3s	−20.0	1.817	1.0		
	3p	−13.3	1.817	1.0		
Au	6s	−10.92	2.602	1.0		
	6p	−5.55	2.584	1.0		
	5d	−15.07	6.163	0.685	2.794	0.5696

For the van der Waals interaction between the surface atoms and the molecule, we used the method described in F. Ample and C. Joachim, Surface Science **602** (2008) 1563–1571, with the standard MM4 parameters

atom	r (Å)	ε (kcal/mol)
C	1.96	0.057
H	1.60	0.017
O	1.76	0.060
S	2.09	0.196
Au	2.43	0.625