

Electronic Supplementary Information for:

Beyond the staple motif: new order at the thiolate-gold interface

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Table S1 Binding energies (eV) of methylthiolate at different adsorption sites on Au(111) with different layers of slab in a (4 × 4) lateral cell. The initial angle between the surface normal and S-C bond is 30°.

Slab thickness	4 layers	5 layers	6 layers
top	-1.64	-1.57	-1.67
bridge	-1.99	-1.96	-2.08
fcc	-1.94	-1.91	-2.02
hcp	Relaxed to bridge	Relaxed to bridge	Relaxed to bridge

Table S2 Binding energies (eV) of methylthiolate at different adsorption sites on Au(100) with different layers of slab in a (4×4) lateral cell.

Slab thickness	4 layers	5 layers	6 layers
top	Relaxed to bridge	Relaxed to bridge	Relaxed to bridge
bridge	-2.41	-2.34	-2.36
square 4-fold hollow	-2.18	-2.08	-2.19

Table S3 Binding energies (eV) of methylthiolate at different adsorption sites on Au(110) with different layers of slab in a (3×4) lateral cell.

Slab thickness	4 layers	5 layers	6 layers
top	Relaxed to short bridge	Relaxed to short bridge	Relaxed to short bridge
long bridge	-2.39	-2.31	-2.36
short bridge	-2.59	-2.47	-2.56
pseudo 3-fold hollow	Relaxed to short bridge	Relaxed to short bridge	Relaxed to short bridge
rectangular 4-fold hollow	Relaxed to short bridge	Relaxed to short bridge	Relaxed to short bridge