Supporting Material

One-dimensional Structures of Three Quinone Molecules on Au(111)

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Figure Captions

Fig. S1. (a) An STM image of NQ molecules on Au(111) surface. Size: 16 × 16 nm^2. Tunneling current: I_T = 0.1 nA. Sample voltage V_S = - 1.18 V. (b) A zoom-in image of the squared region in (a).

Fig. S2. A non-staggered configuration of three (a) AQ, (b) NQ and (c) PQ molecules with simplified electrostatic potential distributions around O and H atoms. The dotted lines indicate possible O···H interactions.

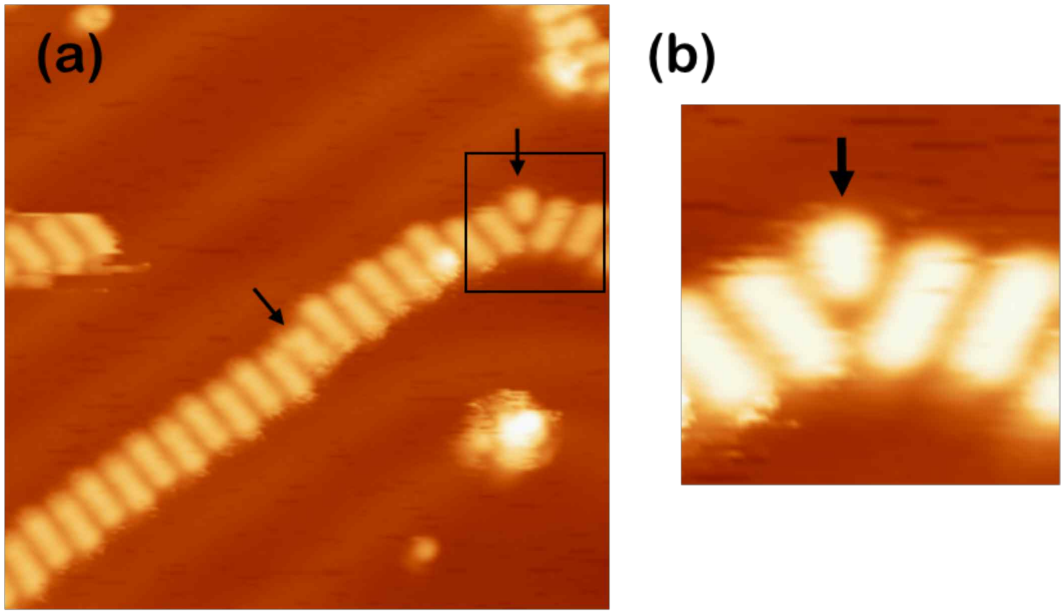


Fig. S1. (a) An STM image of NQ molecules on Au(111) surface. Size : 16 × 16 nm^2, Tunneling current : I_T= 0.1 nA. Sample voltage V_S= - 1.18 V. (b) A zoom-in image of the squared region in (a).

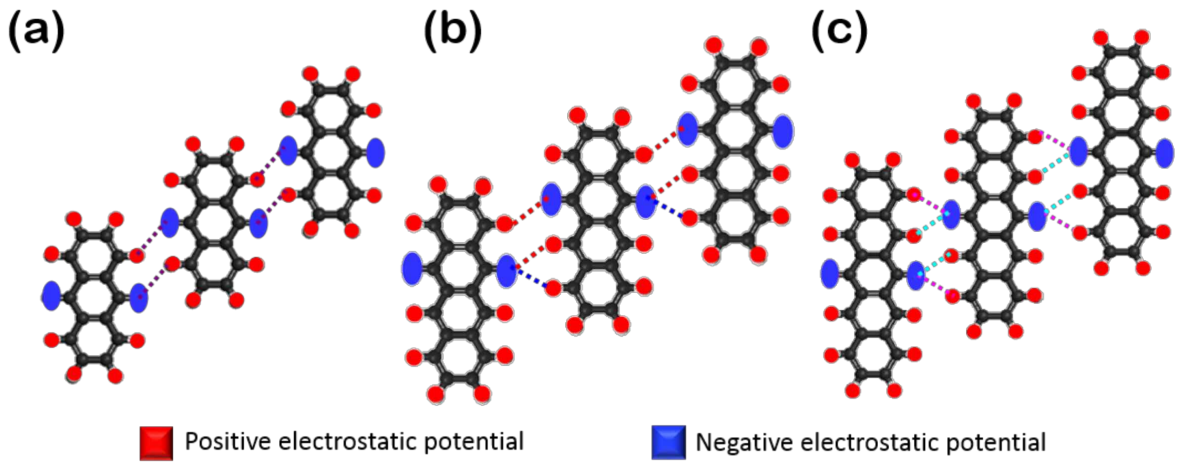


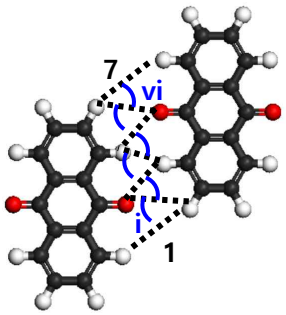
Fig. S2. A parallel configuration of three (a) AQ , (b) NQ and (c) PQ molecules with simplified electrostatic potential distributions around O and H atoms. The dotted lines indicate possible hydrogen bonds.

Table S1. Binding energies for two different configurations

	Staggered configuration	Non-staggered configuration
AQ	221 meV	232 meV
NQ	317 meV	195 meV
PQ	339 meV	353 meV

Optimized bond lengths and angles

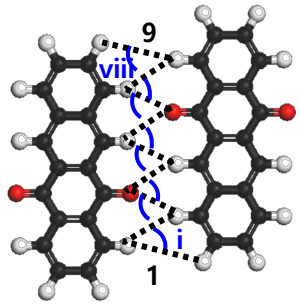
Anthraquinone (AQ),



Bond Number	Bond length (nm)	Angle Number	Angle (◦)
1	0.3803	i	38.907
2	0.2980	ii	50.785
3	0.2550	iii	62.189
4	0.1974	iv	62.182
5	0.2551	v	50.778
6	0.2980	vi	38.907

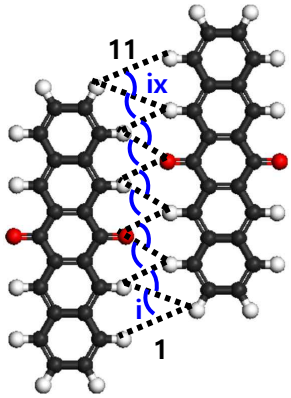
7	0.3803		

Naphthacenequinone (NQ),



Bond Number	Bond length (nm)	Angle Number	Angle (◦)
1	0.3516	i	43.485
2	0.2596	ii	57.841
3	0.2312	iii	59.017
4	0.2455	iv	57.562
5	0.2459	v	57.562
6	0.2455	vi	59.017
7	0.2312	vii	57.841
8	0.2596	viii	43.485
9	0.3516		

Pentacenequinone (PQ)



Bond Number	Bond length (nm)	Angle Number	Angle (◦)
1	0.3705	i	38.716
2	0.3609	ii	43.310
3	0.2454	iii	58.620
4	0.2461	iv	60.477
5	0.2353	v	58.479
6	0.2558	vi	58.479
7	0.2353	vii	60.477
8	0.2461	viii	58.600
9	0.2454	ix	43.294
10	0.3610	x	38.707
11	0.3706		