

## Supporting Information

### Exploration of alkyl chain number and position effects towards 2D self-assembly

Yi Hu, Kai Miao, Li Xu,\* Bao Zha, Xinrui Miao and Wenli Deng\*

College of Materials Science and Engineering, South China University of Technology, Wushan  
Road, Tianhe District, Guangzhou, 510640, P. R. China.

**Tel:** (+86) 020-22236708

**E-mail:** mslxu@scut.edu.cn; wldeng@scut.edu.cn

#### Method for density functional theory (DFT) calculations

We use four unit cells for the calculation of the binding energies for the self-assembled structures.

The hydrogen bonds and van der Waals interactions are calculated separately.

E represent the calculated total energy, then

$E_1$  = total energy for one molecule

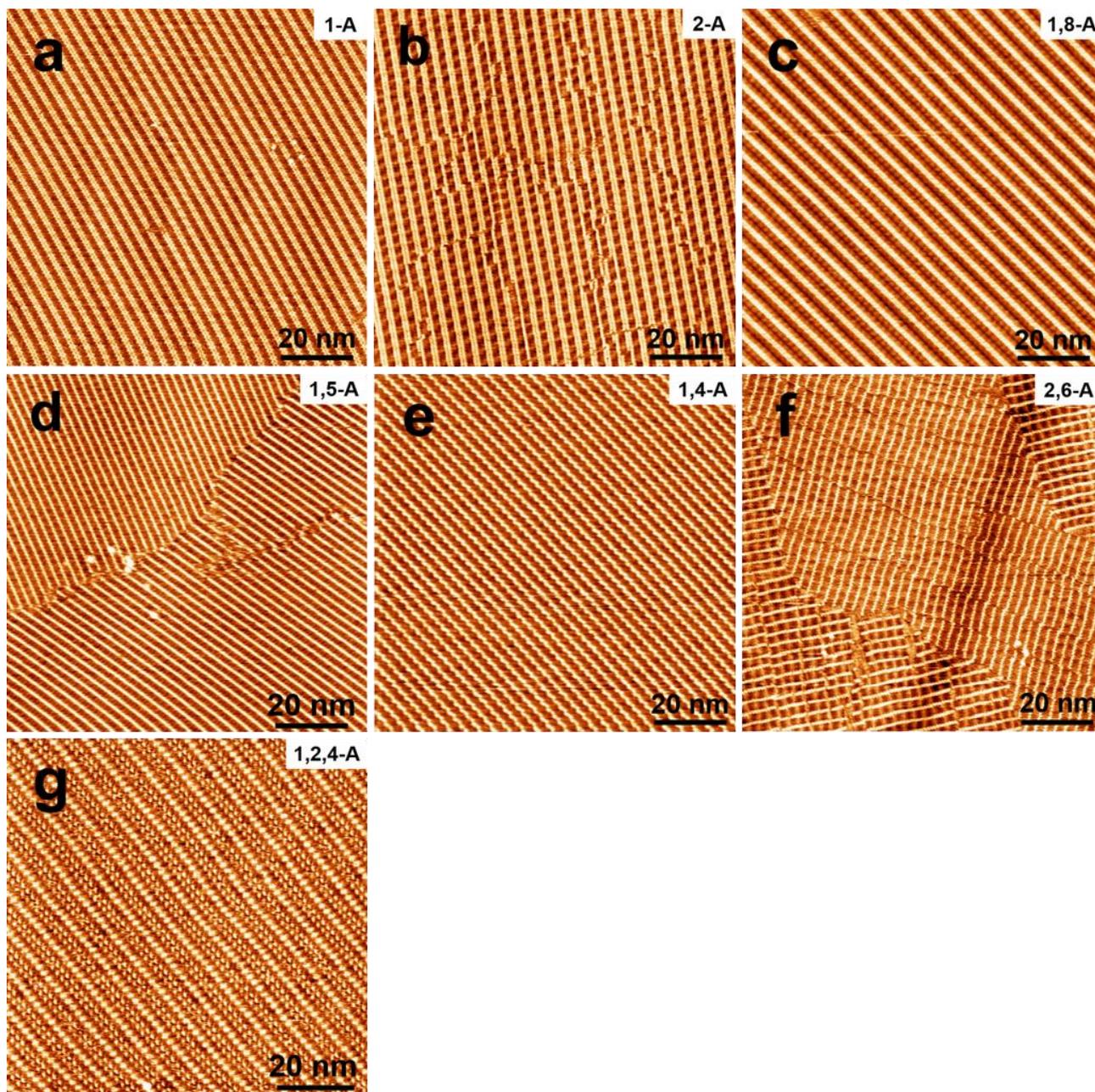
$E_2$  = total energy for the four unit cells

N = number of molecules in the unit cell

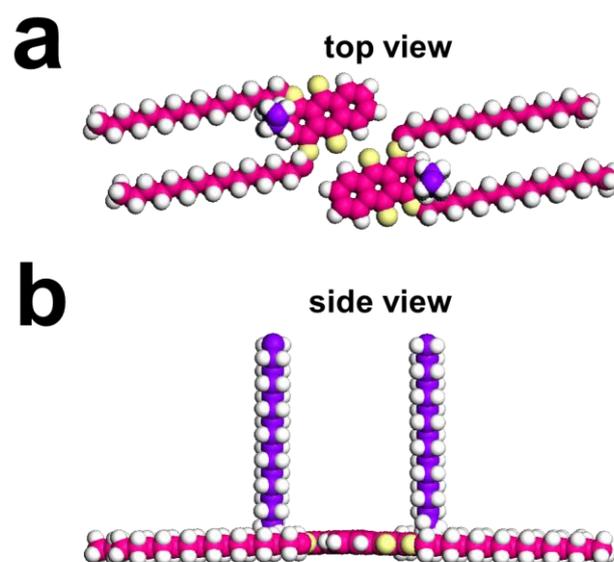
$\Delta E$  = the binding energy

$\Delta E = E_2 - 4N \cdot E_1$

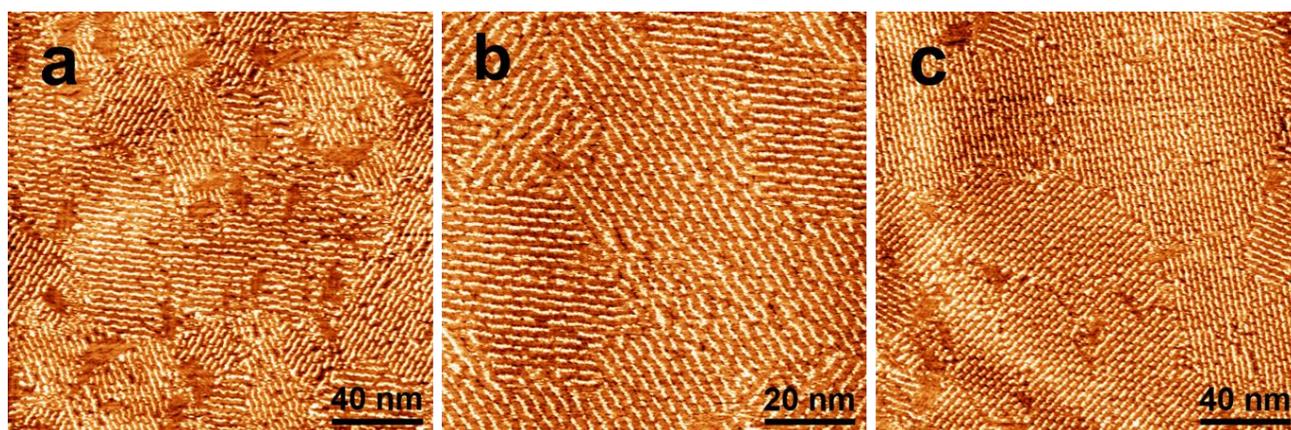
## Results



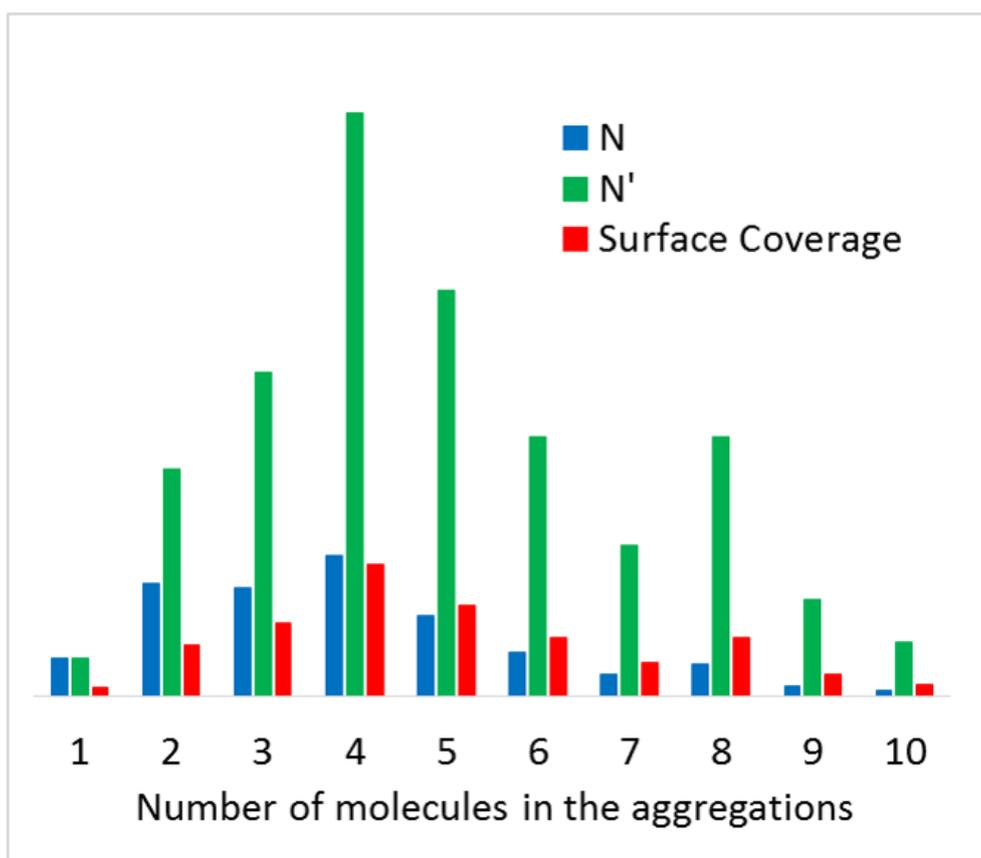
**Fig. S1** High-resolution STM images for (a) 1-A, (b) 2-A, (c) 1,8-A, (d) 1,5-A, (e) 1,4-A, (f) 2,6-A and (g) 1,2,4-A at the 1-octanoic acid/HOPG interface, showing the Linear I, Linear II, Linear III, Linear IV, Zigzag, Linear V and Dimer-Linear structures, respectively. Imaging conditions:  $I_t = 450\text{--}700$  pA,  $V_{\text{bias}} = 550\text{--}900$  mV.



**Fig. S2** Structural model for the dimer in Dimer-Linear structure for 1,2,4-A molecules from the (a) top view and (b) side view. In the Linear rows, the three chains belong to one 1,2,4-A molecule are fully interdigitated with the chains from the adjacent rows. However, in the dimer rows, we can only observe two chains, which means the other chain is directing to the liquid phase.



**Fig. S3** Large-scale STM images for 1,2,3-A at the 1-octanoic acid/HOPG interface. Scanning conditions:  $I_t = 610$  pA,  $V_{\text{bias}} = 780$  mV.



**Fig. S4** Surface coverage distribution of aggregations with different number of molecules (measuring area:  $50 \times 50 \text{ nm}^2$ ).  $N$  represents number of a certain aggregation.  $N'$  represents total number of molecules in a certain aggregation.

**Table S1.** Phase-transition temperatures and UV absorption peaks for the anthraquinone derivatives.

	mono-		bis-			tri-		
	1-A	2-A	1,8-A	1,5-A	1,4-A	2,6-A	1,2,4-A	1,2,3-A
phase-transition temperature ( $^{\circ}\text{C}$ )	99	89	109	104	97	111	101	69
$\lambda_{\text{max}}$ (nm)	380	370	385	420	380	350	405	365