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Two Solvent-induced variable Host-Guest Two-dimensional Binary Frameworks Mediated by Hydrogen Bonding

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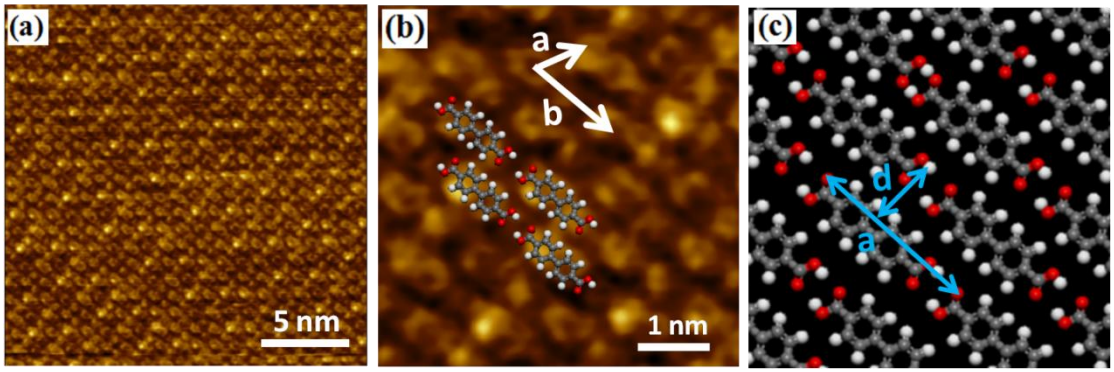

Fig. S1. (a) Large scale STM image of the BDA monolayer at the heptanoic acid/HOPG interface (*I*=0.42 nA, *V* = -0.65 V). (b) High-resolution image of the BDA monolayer at the heptanoic acid/HOPG interface (*I*=0.37 nA, *V* = -0.67 V). (c) Model of the BDA molecules, the molecule-molecule distance along the long molecular axis is found to be a=1.41±0.02nm and d=0.62±0.02nm in the orthogonal direction.

Fig.S1 shows the STM well-ordered and close-packed structure of the BDA molecule at the heptanoic acid/HOPG interface. A DFT-based geometry optimization of an isolated molecule yields a dihedral angle of 32^0 between the otherwise planner phenyl moieties.[1] Close examination of the image in Figure 1S(b) reveals that the one-dimensional chains formed by molecular head-to-tail coupling of linear O-H ⋯ O hydrogen bonds between self-complementary carboxylic end groups. A proposed model for the molecular arrangement could be proposed according to the STM image (Figure 1S(c)). The molecule-molecule distance along the long molecular axis is found to be *a*=1.41±0.02nm and *d*=0.62±0.02nm in the orthogonal direction.

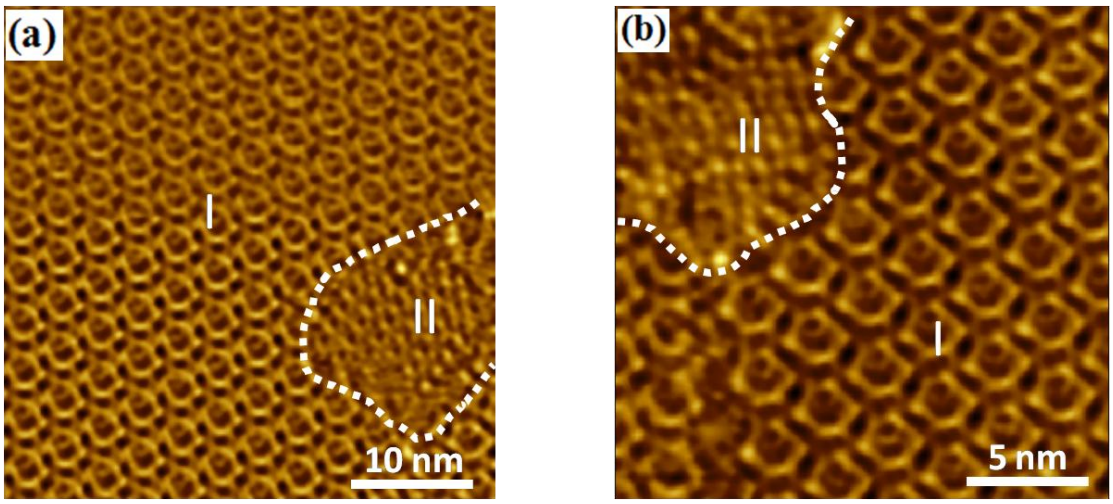

Fig. S2. (a) STM image of structures I and II co-adsorbed on heptanoic acid/HOPG interface (I = 0.35 nA, V = -0.62 V); (b) STM image of TMA/TPA/$AgNO_3$ co-adsorption structure on heptanoic acid/HOPG interface. (I = 0.28 nA, V = -0.69 V).

Fig. S2 shows the STM flower structure of TMA and BDA molecules dissolved in heptanoic acid with the molar ratio of TMA: BDA is just to 3:2, two distinct structures labeled as I and II can be observed on the same surface area with the white lines as the indicators of phase-separated boundaries. It is obvious that the structure of the flower network has been significantly changed by introducing redundant BDA molecules, and the spots in the structure I holes may be BDA molecules. Structure II is the self-assembly of BDA structure.

Table S1. The lattice parameters for the 2D BDA networks

	Unit parameters		
	a (nm)	*b* (nm)	α (^{0})
Structure I (zigzag chain-like)	1.2 ± 0.1nm	1.3 ± 0.1nm	62 ± 1^0
Structure II (lateral coupling)	1.1 ± 0.1nm	1.5 ± 0.1nm	58 ± 1^0
Structure III (head-to-tail)	0.7 ± 0.1nm	1.4 ± 0.1nm	45 ± 1^0