

Supporting Information

Coronene Guest Molecule Selectivity in the Host Templates Formed by Hydrogen Bond and Van der Waals Force at Liquid/Solid Interface

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S1. Acronyms table

Table S1 The definition of Acronyms in the main text.

Acronyms	Full name
H ₆ PDB	1,3,5-tris(4-(3,5-dicarboxyphenyl) diphenyl) benzene
H ₆ PAB	1,3,5-tris (4-(3,5-dicarboxyphenylacetylene) phenyl) benzene
COR	1,3,5-tris (4-(3,5-dicarboxyphenylacetylene) phenyl) benzene
HPB	Hexaphenylbenzene derivatives
H ₄ ETTC	4',4'',4''',4''''-(ethene-1,1,2,2-tetrayl) tetrakis-([1,1'-biphenyl]-3-carboxylic acid)
H ₈ ETTB	4',4'',4''',4''''-(ethene-1,1,2,2-tetrayl) tetrakis([1,1'-biphenyl]-3,5-dicarboxylic acid)

S2. Sample Preparation

Table S2 The information of all the samples used in the experiment.

Sample	Obtained from	Purity
H ₆ PDB	Jilin Chinese Academy of Sciences-Yanshen Technology Co., Ltd.	98%
H ₆ PAB	Jilin Chinese Academy of Sciences-Yanshen Technology Co., Ltd.	98%
HPB	synthesized by the previous reference	98%
COR	Beijing HWRK Chemical Corporation	98%
1-heptanoic acid (HA)	J&K Scientific	98%

All the samples were at 98% purity and used directly without further purification. All the samples were dissolved in HA solvent. The concentrations of H₆PDB, H₆PAB and HPB solution were 10% of their saturated concentrations. COR/HA solution was prepared in C1 = 10⁻⁵ mol·L⁻¹, C2 = 8 × C1, and saturated concentration (C3) respectively. H₆PAB and HPB solution was premixed in 1:1 ratio. The volume of COR added in-suit was the same as the premixed solution.

S3. Large scale STM image of H₆PDB and H₆PAB co-assembled with saturated COR/HA solution(C3)

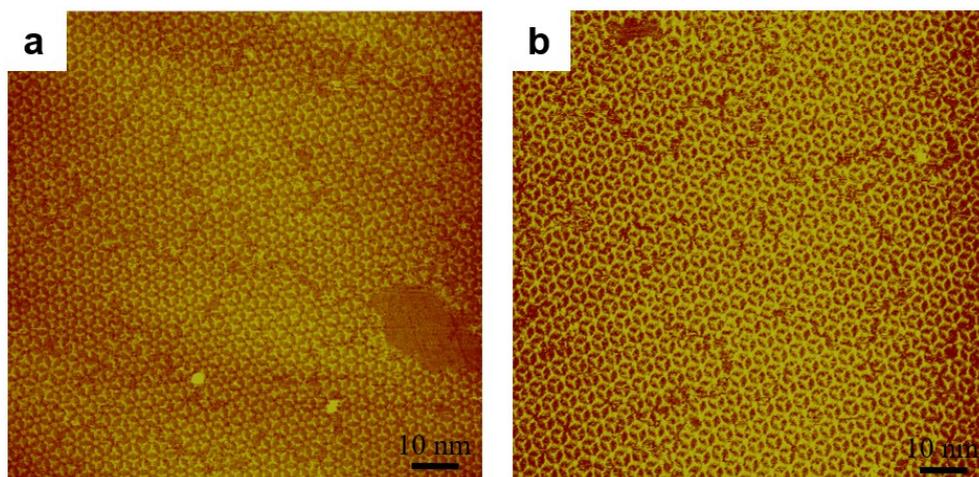


Figure S1. (a) Large scale STM image of H₆PDB/COR(C3) co-assembled structure ($I_{\text{set}} = 259.4$ pA, $V_{\text{bias}} = 809.9$ mV, $100 \text{ nm} \times 100 \text{ nm}$); (b) Large scale STM image of H₆PAB/COR(C3) co-assembled structure ($I_{\text{set}} = 268.6$ pA, $V_{\text{bias}} = 806.3$ mV, $100 \text{ nm} \times 100 \text{ nm}$).

S4. High resolution STM image and molecular model of HPB self-assembled structure and HPB/COR co-assembled structure

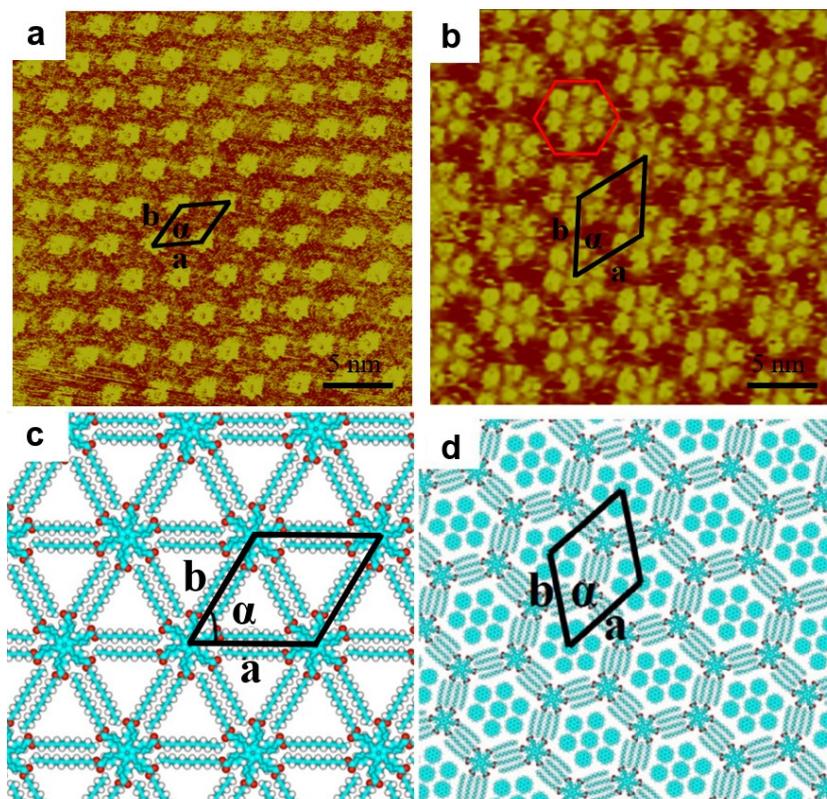


Figure S2. (a) High resolution STM image of HPB self-assembled structure ($I_{\text{set}} = 271$ pA, $V_{\text{bias}} = 799$ mV, $25 \text{ nm} \times 25 \text{ nm}$); (b) High resolution STM image of HPB/COR(C3) co-assembled structure ($I_{\text{set}} = 198.4$ pA, $V_{\text{bias}} = 739.7$ mV, $25 \text{ nm} \times 25 \text{ nm}$); (c) (d) Proposed models of the structures in (a) and (b) respectively.