

Electronic Supplementary Information

## **The self-assembly of a pair of low symmetric tetracarboxylic acid molecules and their co-assembly with bridging molecule at the liquid–solid interface**

Siqi Zhang,<sup>a,b</sup> Jianqiao Li,<sup>b</sup> Linlin Gan,<sup>b</sup> Lin Ma,<sup>b</sup> Wei Ma,<sup>d</sup> Min Zhang,<sup>\*,a</sup> Faliang Cheng,<sup>\*,a</sup> Ke Deng<sup>\*,b</sup> and Qingdao Zeng<sup>\*,b,c</sup>

<sup>a</sup>Guangdong Engineering and Technology Research Center for Advanced Nanomaterials, School of Environment and Civil Engineering, Dongguan University of Technology, Dongguan 523808, China.

<sup>b</sup>CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology (NCNST), Beijing 100190, China.

<sup>c</sup>Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.

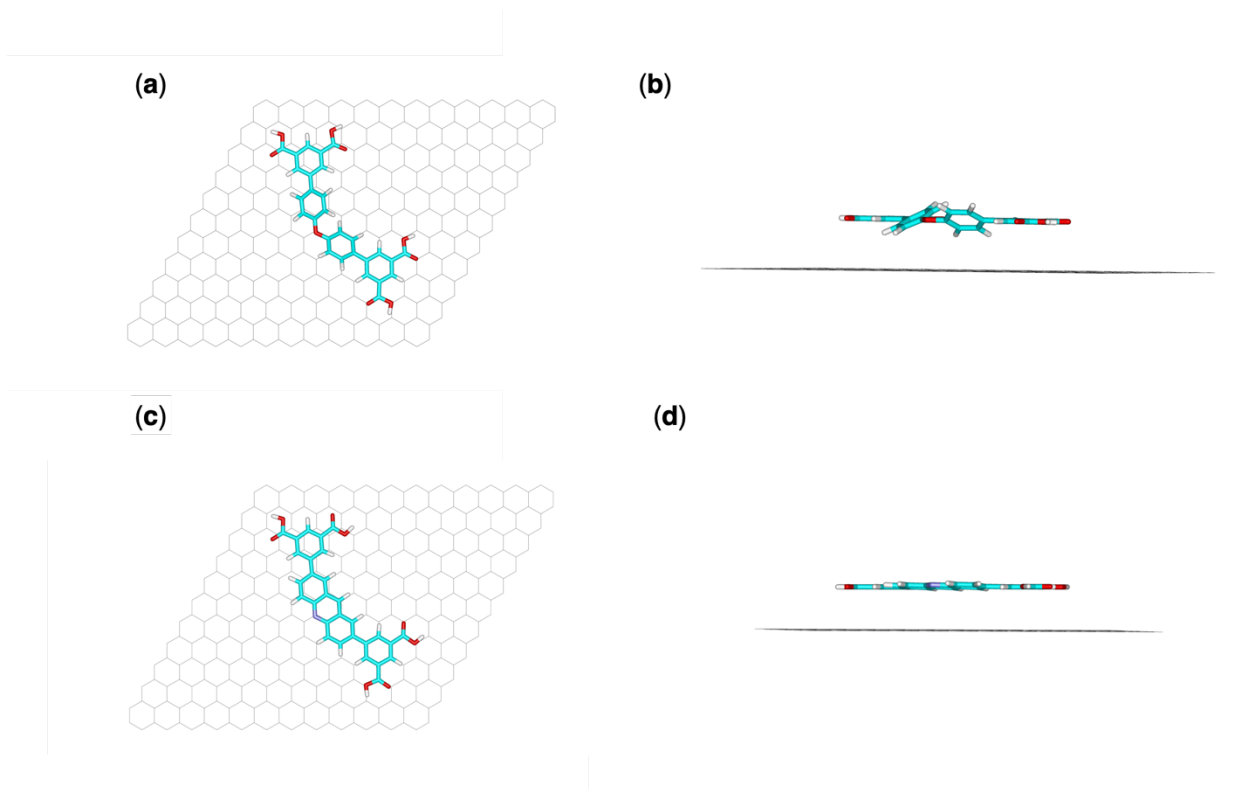
<sup>d</sup>State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China.

**\*Corresponding author E-mail:** mindear@dgut.edu.cn (M. Z.); chengfl@dgut.edu.cn (F. C.); kdeng@nanoctr.cn (K. D.); zengqd@nanoctr.cn (Q. Z.).

Table of Contents:

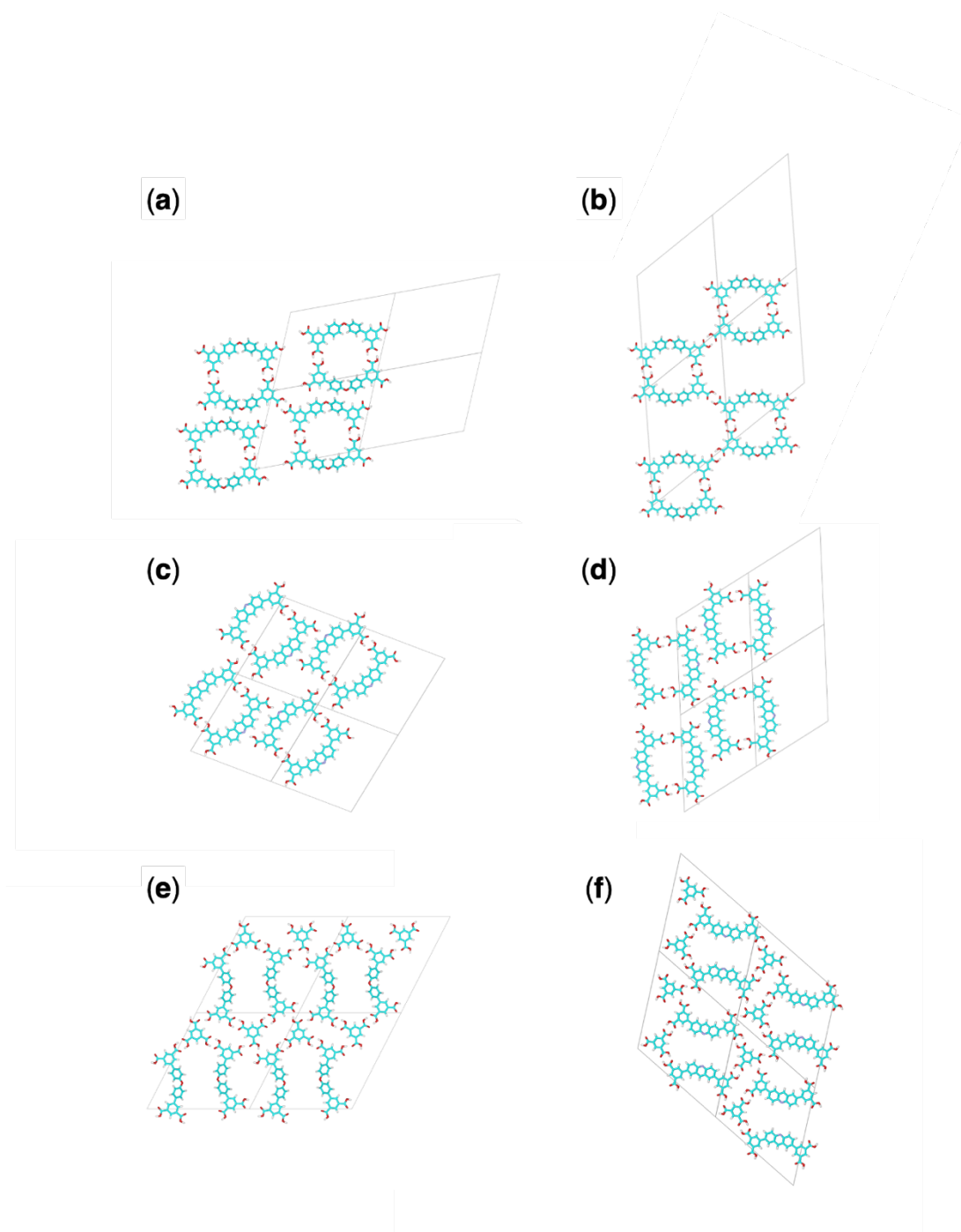
1	DFT simulated single molecular models.....	S3
2	Details of DFT simulated molecular models of the assembled structures .....	S4

1 DFT simulated single molecular models.



**Fig. S1** DFT simulated single molecular models on the graphite surface. (a) Top view of H<sub>4</sub>OBDB. (b) Side view of H<sub>4</sub>OBDB. (c) Top view of H<sub>4</sub>ADDI. (d) Side view of H<sub>4</sub>ADDI.

2 Details of DFT simulated molecular models of the assembled structures.



**Fig. S2** Details of DFT simulated molecular models of the assembled structures on the graphite surface. Molecular model of (a) H<sub>4</sub>OBDB\_stru1, (b) H<sub>4</sub>OBDB\_stru2, (c) H<sub>4</sub>ADDI\_stru1, (d) H<sub>4</sub>ADDI\_stru2, (e) H<sub>4</sub>OBDB-TMA, (f) H<sub>4</sub>ADDI-TMA.