SUPPORTING INFORMATION

STM/STS Study of Site-selective Adsorption of C70 Molecules onto Arc-shaped BODIPY Molecular-Networks

Jing Xu,[a,b] Wenxu Liu,[b,c] Yanfang Geng[a,b] Ke Deng,*[a,b] Chuanlang Zhan,*[c] Qingdao Zeng*[a,b]

a. CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology (NCNST), Beijing 100190, P. R. China.

b. University of Chinese Academy of Sciences, Beijing 100049, P. R. China.

c. Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences.

LIST OF CONTENTS

1. Calculated band structures and partial density of states of the assemblies.
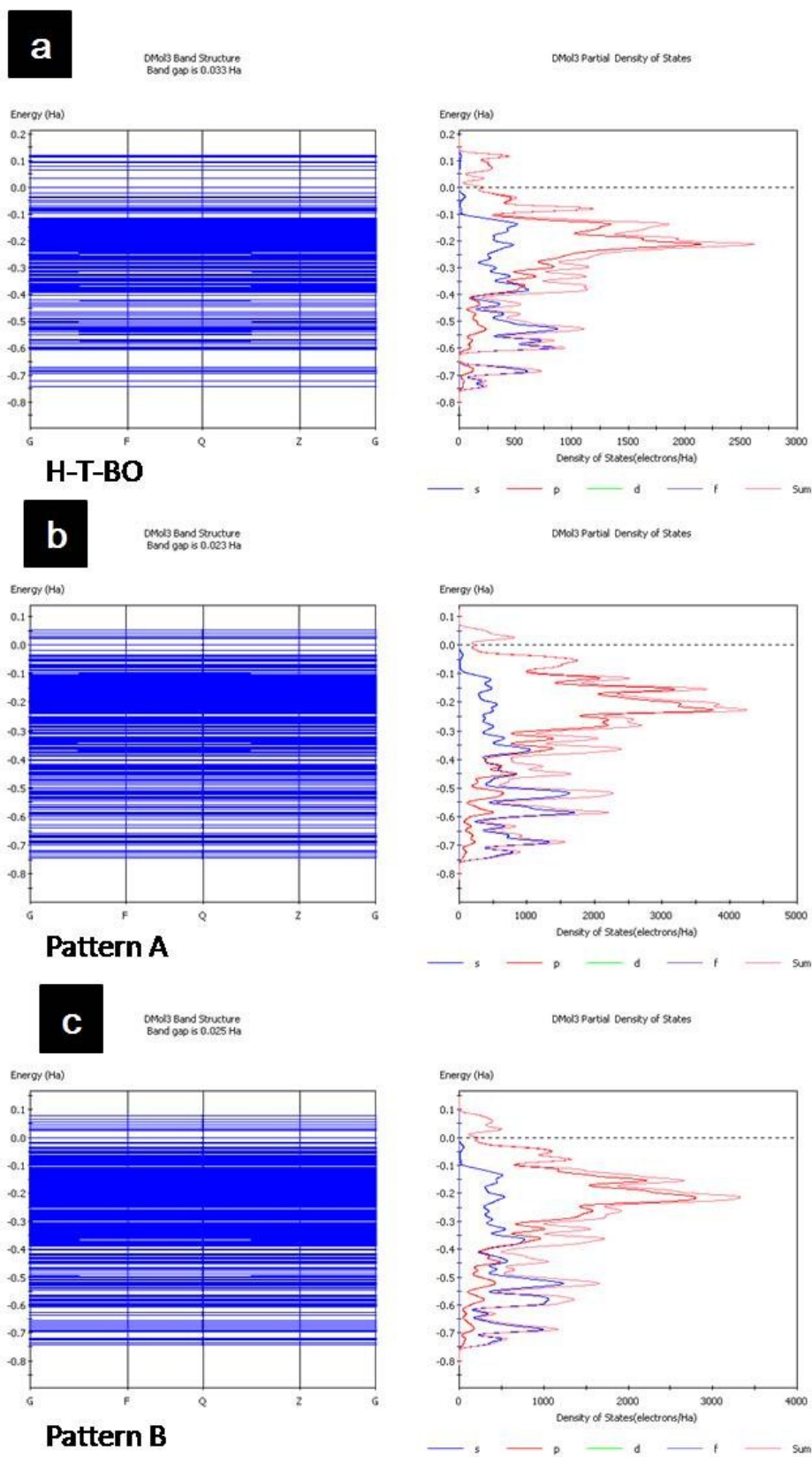

Figure S1. Calculated band structures and partial density of states of (a) H-T-BO, (b) Pattern A, and (c) Pattern B.

It is known that 1 Ha is equivalent to 27.2116 eV.

For H-T-BO, the calculated band gap of 0.033 Ha can be converted to $0.033 \times 27.2116 \approx 0.90$ eV.

For Pattern A, the calculated band gap of 0.023 Ha can be converted to $0.023 \times 27.2116 \approx 0.63$ eV.

For Pattern B, the calculated band gap of 0.025 Ha can be converted to $0.025 \times 27.2116 \approx 0.68$ eV.

2. The Split STM image

The Split STM image (Figure S2) are recorded by changing the tunneling parameters from adsorbate conditions (high voltage, low current) to graphite conditions (low voltage, high current) during the scan of the image frame. Since the standard unit cell parameters of graphite are known very precisely (a = 2.46Å, b = 2.46 Å, α = 60°), the STM image can be calibrated with these values and the unit cell of the adsorbate layer can be determined. Figure **S2.b** showed the enlarged STM image of HOPG in Figure **S2.a**. The experimental values of unit cell parameters of

HOPG are a = 2.49±0.20 Å, b = 2.50±0.20 Å, α = 60.59°±2.00°. Direction of vector

a and b was marked out in Figure **S2.b**.

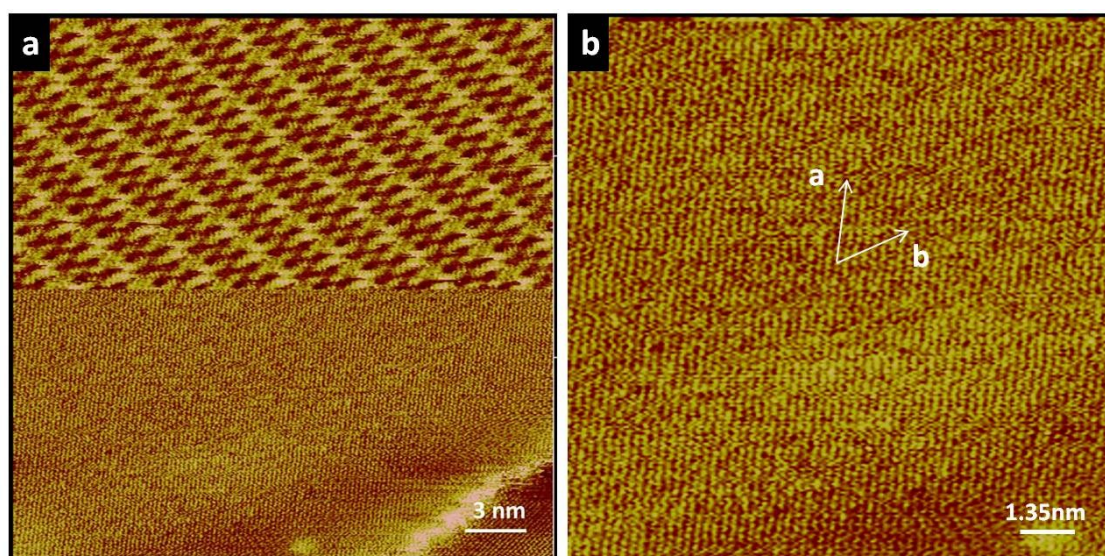**Figure S2**. (a)Split image: the upper part shows the adsorbate layer H-T-BO, I_{set} = 299.1pA, V_{bias} = 599.1 mV, scan rate = 6.1 Hz; the lower part shows the underlying substrate (HOPG), I_{set} = 699.1pA, V_{bias} = 59.1 mV, scan rate = 6.1 Hz. (b) Enlarged STM image of HOPG in (a).