

# Selective Adsorption of Coronene atop Polycyclic Aromatic

## Diimide Monolayer Investigated by STM and DFT

Yanfang Geng,<sup>†a</sup> Shuai Wang,<sup>†a</sup> Mengqi Shen,<sup>a</sup> Ranran Wang,<sup>b</sup> Xiao Yang,<sup>b</sup> Bin Tu,<sup>\*a</sup>

Dahui Zhao,<sup>\*b</sup> Qingdao Zeng<sup>\*a</sup>

<sup>a</sup> CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology (NCNST), 11 ZhongguancunBeiyitiao, Beijing 100190, P. R. China

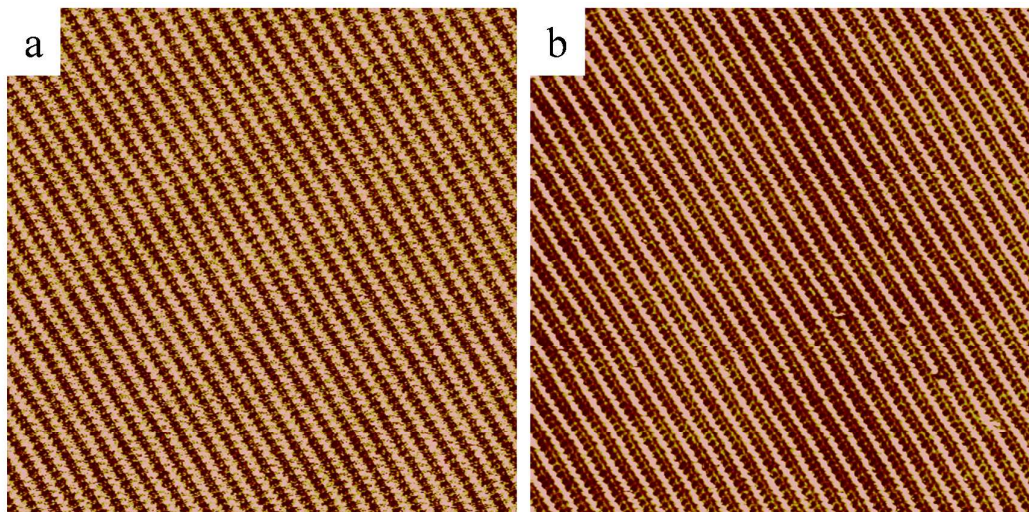
<sup>b</sup> Beijing National Laboratory for Molecular Sciences, the Key Laboratory of Polymer Chemistry and Physics of the Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China.

<sup>†</sup> These authors equally contributed to this work.

E-mail: [tub@nanoctr.cn](mailto:tub@nanoctr.cn); [dhzhao@pku.edu.cn](mailto:dhzhao@pku.edu.cn); [zengqd@nanoctr.cn](mailto:zengqd@nanoctr.cn)

**Table S1.** Experimental (Exp.) and calculated (Cal.) unit-cell parameters of PAI1, PAI1+Cor, PAI2, PAI6 and PAI8 arrays.

		PAI1	PAI1+Cor	PAI2	PAI6	PAI8
$a$ (nm)	Exp.	$2.7 \pm 0.1$	$2.9 \pm 0.1$	$2.8 \pm 0.1$	$2.7 \pm 0.1$	$2.8 \pm 0.1$
	Cal.	2.78	2.90	2.62	2.94	2.96
$b$ (nm)	Exp.	$1.1 \pm 0.1$	$1.3 \pm 0.1$	$1.1 \pm 0.1$	$1.0 \pm 0.1$	$1.0 \pm 0.1$
	Cal.	1.16	1.28	1.20	1.06	1.22
$\alpha$ ( $^\circ$ )	Exp.	$92 \pm 2$	$99 \pm 2$	$82 \pm 2$	$82 \pm 2$	$88 \pm 2$
	Cal.	92	99	82	82	88



**Figure S1.** Large-scale STM images (70 nm  $\times$  70 nm) of PA11 self-assembled structures (a) and that incorporating coronene in PA11 preassembled structure (b). Tunneling condition: (a)  $I_{\text{set}} = 296.0$  pA,  $V_{\text{bias}} = 557.6$  mV; (b)  $I_{\text{set}} = 296.0$  pA,  $V_{\text{bias}} = 675.0$  mV.