

## Supporting Information

### **Investigating Non-covalent Interactions of Molecular Self-assembly with the Association of Aromatic Structures in Pyrene-4,5,9,10-tetraone and Phenanthrene-9,10-dione Molecules by Scanning Tunneling Microscopy**

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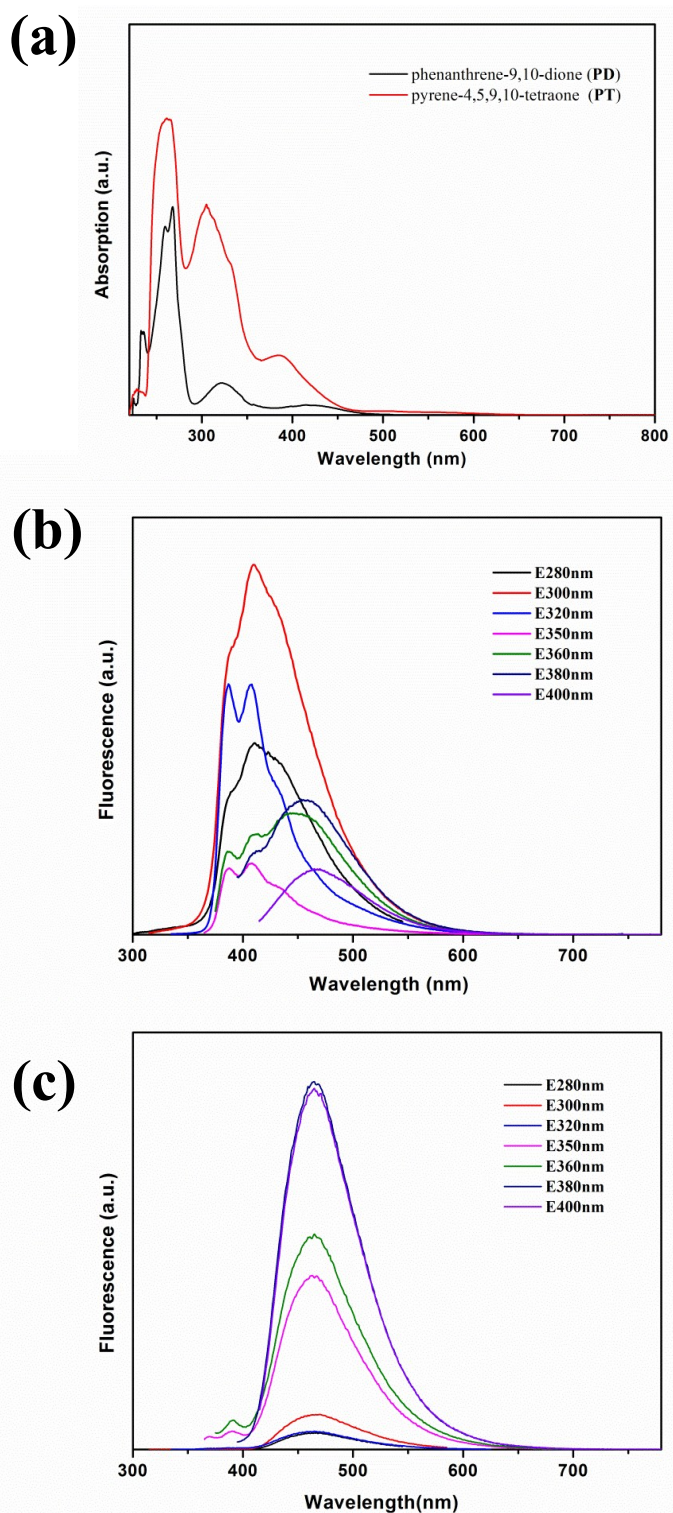
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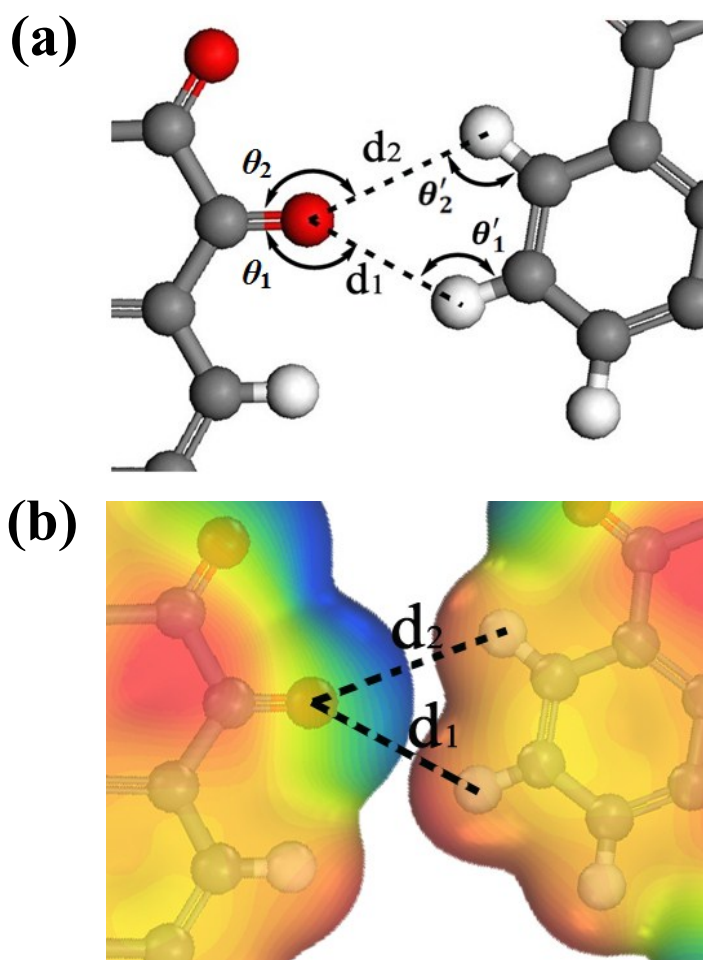
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**Fig.S1** (a) Absorption spectra with baseline of **PD** and **PT** dissolved in chloroform; (b) and (c) fluorescent spectra of **PD** and **PT** dissolved in chloroform, respectively.

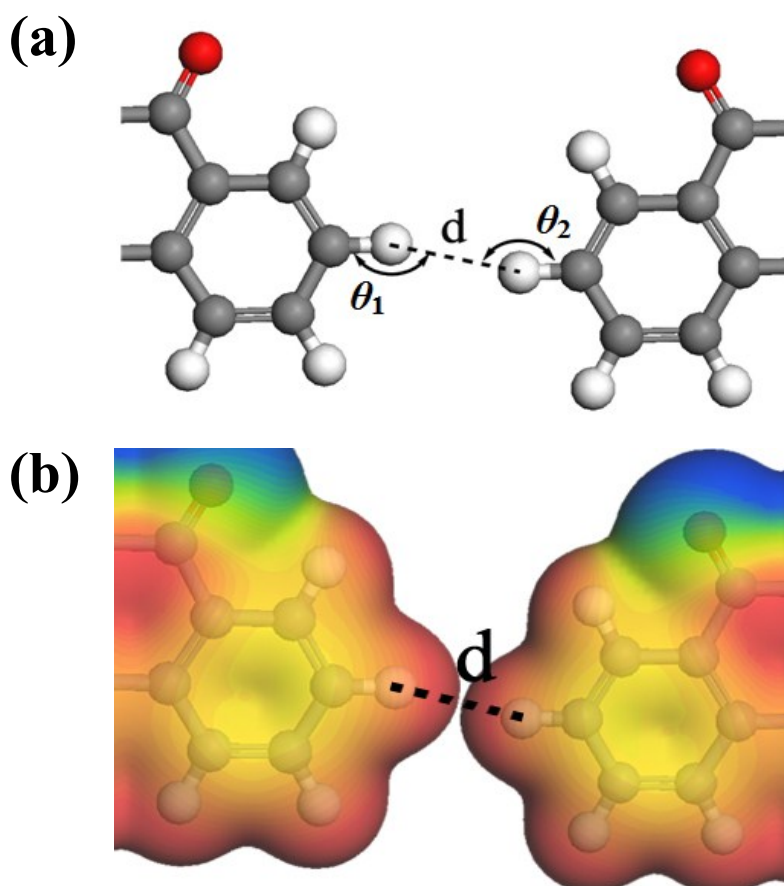


**Fig.S2** (a) Schematic defining the intermolecular bond distances, angle  $\theta_1$  around electrophilic H atoms and angle  $\theta_2$  around the nucleophilic O atoms in the chevron structure formed by **PT** molecules. (b) Measured bond distances  $d$  for intermolecular bonds and measured  $\theta$  values in calculated structures.



<i>Distance</i> $d_1$ (nm)	<i>Angle</i> $\theta_1$ (°)	<i>Angle</i> $\theta'_1$ (°)	<i>Distance</i> $d_2$ (nm)	<i>Angle</i> $\theta_2$ (°)	<i>Angle</i> $\theta'_2$ (°)
0.25	170	152	0.34	148	107

**Fig.S3** (a) Schematic defining the intermolecular bond distance  $d$ , angle around H atoms located at both ends of **PD** molecules. (b) Measured bond distances for intermolecular bonds and measured  $\theta$  values in calculated structures.



<i>Distance <math>d</math>(nm)</i>	<i>Angle <math>\theta_1</math>(°)</i>	<i>Angle <math>\theta_2</math>(°)</i>
0.25	155	155

**Fig.S4** The typical STM image with high resolution obtained in PT and PD binary assembly experiment.

