

**Self-assembly of discotic liquid crystalline molecule-modified gold nanoparticles:  
control between 1D and hexagonal ordering induced by solvent polarity**

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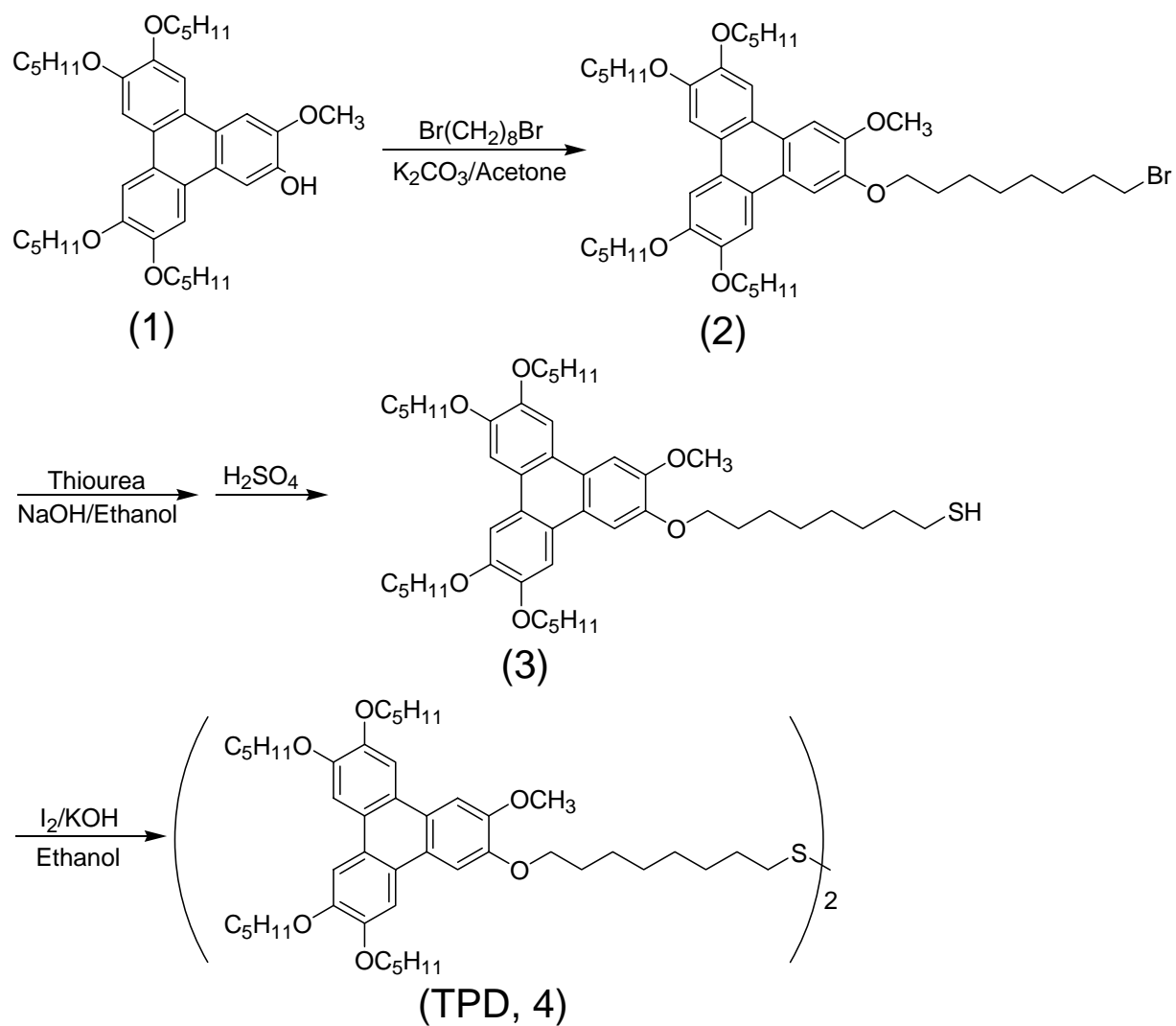
**Electronic Supplementary Information**

**Table S1** <sup>1</sup>H-NMR chemical shifts of TP moieties<sup>a)</sup>

Proton	<sup>1</sup> H NMR chemical shift /ppm			
	Compounds			
	TPD	Au-TP1	Au-TP2	Au-TP3
Ar-H <sup>b)</sup>	7.79-7.88 (m)	7.01 (b)	6.88 (b)	6.80 (b)
Ar-OCH <sub>3</sub> <sup>b)</sup>	4.08 (s)	3.70 (b)	3.62 (b)	3.53 (b)

a) The values of chemical shifts refer to Fig. S1.

b) Ar indicates the triphenylene flume of TPD illustrated in Scheme S1.



**Scheme S1** Preparation of TPD.

### **Synthesis of 2-(8-hydroxy-3-methoxy-6, 7, 10, 11-tetrakis-pentyloxy triphenylene (1)**

The compound was synthesized based on reference<sup>1</sup>(see the footnote of this page).

### **Synthesis of 2-(8-bromo-octoxy)-3-methoxy-6, 7, 10, 11-tetrakis-pentyloxy-triphenylene (2)**

Compound **1** (2.0 g, 3.23mmol), potassium carbonate (1.2 g, 8.7 mmol), 1, 8-dibromooctane (10.5 g, 38.6 mmol) and 50 mL acetone were mixed together, then heated to reflux for 24 h. Cooled down to room temperature (rt) then filtered. The solvent was removed under vacuum to produce a colorless liquid. This liquid was added into 100 mL ethanol, cooled to 0 °C for 2 h, filtered and washed with cool ethanol. The cake was recrystallized in 60 mL ethanol. The desired product **2** was obtained as a white solid. (2.3g, 88% yield).

*Characterization for compound 2:* <sup>1</sup>H NMR (500M, CDCl<sub>3</sub>): δ7.86-7.80 (m, 6H), 4.24 (t, 10H), 4.10 (s, 3H), 3.42 (t, 2H), 2.00-1.81 (m, 12H), 1.61-1.40 (m, 24H), 0.98 (t, 12H). FT-IR (KBr) 2954 (Ar-H), 2929, 2858, 1618 (C=C), 1517, 1436, 1388, 1261, 1054 (C-O), 837 cm<sup>-1</sup>. Anal. Calcd for C<sub>47</sub>H<sub>69</sub>BrO<sub>6</sub>: C, 69.70; H, 8.59. Found: C, 70.29; H, 9.01.

### **Synthesis of 2-(8-thio-octoxy)-3-methoxy-6, 7, 10, 11-tetrakis-pentoxy-triphenylene (3)**

Compound **2** (2.0g, 2.47 mmol), thiourea (0.47 g, 6.18 mmol) and 110 mL ethanol were mixed under nitrogen, then heat to reflux and kept for 6-12 h till reaction finished, detected by TLC. After it was finished, it was cooled to rt then sodium hydroxide solution (2.5 g, 10%) was added. After refluxing for approximate 4 h, the system was cooled to rt and the pH was adjusted to 7 with diluted sulfuric acid. The system was cooled to 0 °C for 2 h, filtered and washed with water, and recrystallized in 50 mL ethanol. The intermediate product **3** was obtained as a yellow solid without further purifying. (1.51g, 80.3% yield).

*Characterization for compound 3:* <sup>1</sup>H NMR (500M, CDCl<sub>3</sub>): δ7.84-7.81 (m, 6H), 4.24 (t, 10H), 4.10 (s, 3H), 2.54 (q, 2H), 1.95 (m, 12H), 1.59-1.35 (m, 24H), 0.98 (t, 12H). FTIR (KBr) 3448 (S-H), 2954 (Ar-H), 2929, 2858, 1618 (C=C), 1517, 1436, 1390, 1261, 1054 (C-O), 837 cm<sup>-1</sup>. Anal. Calcd for C<sub>47</sub>H<sub>70</sub>O<sub>6</sub>S: C, 73.97; S, 4.20; H, 9.25. Found: C, 74.37; S, 4.39, H, 8.82.

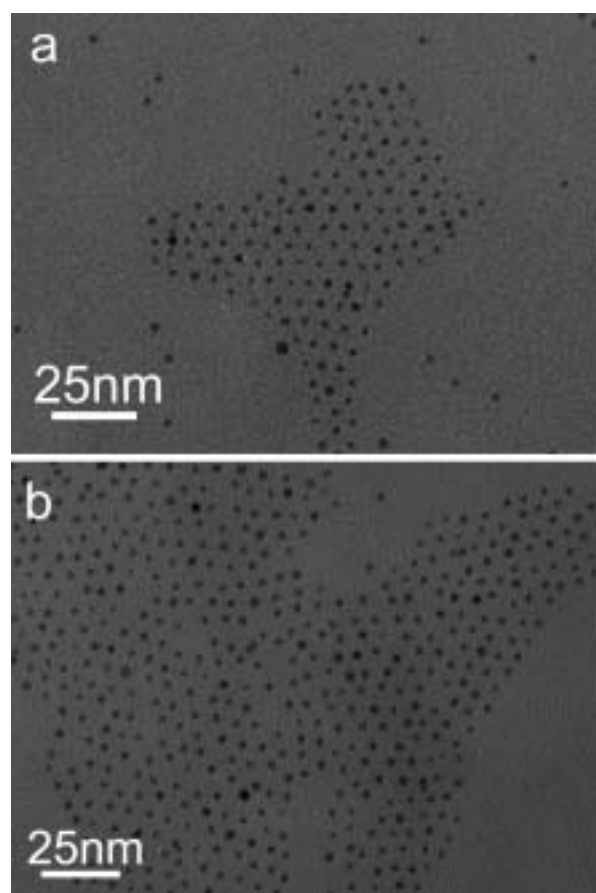
### **8-(3-methoxy-6, 7, 10, 11-tetrakis-pentyloxy-triphenylene-2-yloxy)-octanyl disulfide (TPD, 4)**

Compound **3** (1.5g, 2.0 mmol), 30 mL methanol, 100mL ethanol, 1.5g potassium hydroxide (1.5g, 10%) and iodine (0.31g, 1.2mmol) were mixed in a 500 mL flask, then heated to reflux overnight. After it was cooled to rt and the solvent was removed under vacuum, it was dissolved into 100 mL ethyl acetate, and washed with 50 mL water twice. The solvent was removed and the compound was recrystallized by 60 mL ethanol. The final product **4** was obtained as a pale yellow solid. (1.2g, 80% yield).

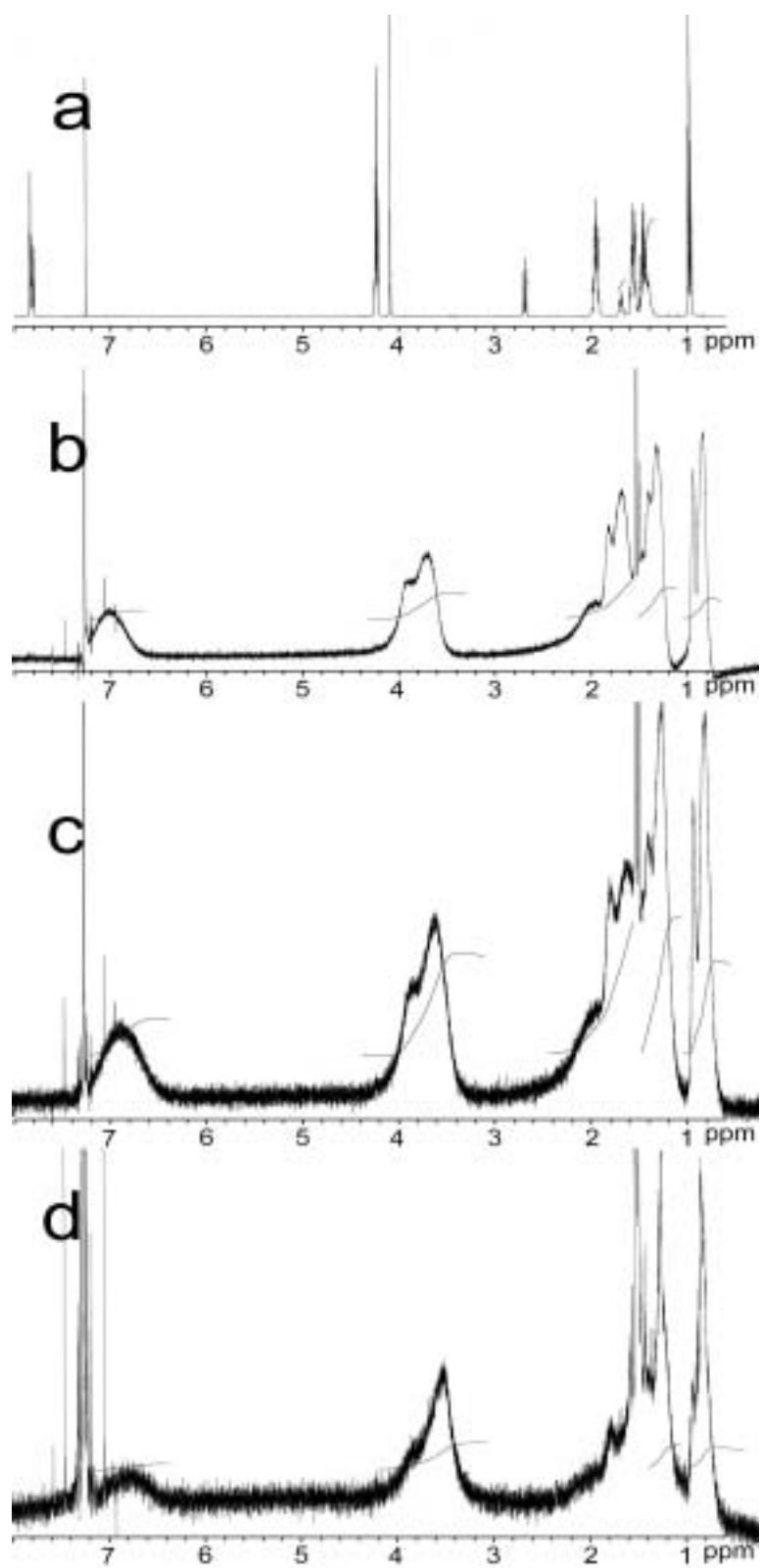
*Characterization for compound 4:* <sup>1</sup>H NMR (500M, CDCl<sub>3</sub>) as shown in figure S1: δ7.84-7.80 (m, 12H), 4.23 (t, 20H), 4.09 (s, 6H), 2.69 (t, 4H), 1.98-1.92 (m, 20H), 1.71-1.68 (m, 4H), 1.60-1.53 (m, 22H), 1.49-1.38 (m, 28H), 0.99 (t, 24H). FTIR (KBr) 2954 (Ar-H), 2927, 2858, 1618 (C=C), 1517, 1508, 1434, 1263, 1167, 1051 (C-O), 835 cm<sup>-1</sup>. Anal. Calcd for C<sub>94</sub>H<sub>138</sub>O<sub>12</sub>S<sub>2</sub>: C, 74.10; S, 4.21; H, 9.13. Found: C, 74.33; S, 3.96; H, 8.85

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<sup>1</sup> C. Ba, Z. Shen, H. Gu, G. Guo, P. Xie, R. Zhang, *Liq. Cryst.*, 2003, **30**, 391.



**Fig. S1** TEM images of (a) Au-TP2 and (b) Au-TP3 prepared in toluene.



**Fig. S2**  $^1\text{H-NMR}$  of (a) TPD, (b) Au-TP1, (c) Au-TP2, and (d) Au-TP3 in  $\text{CDCl}_3$  at 500 MHz.