Electronic Supplementary Information for-

Charge transport in phenazine–fused triphenylene discotic mesogens doped with CdS nanowires†

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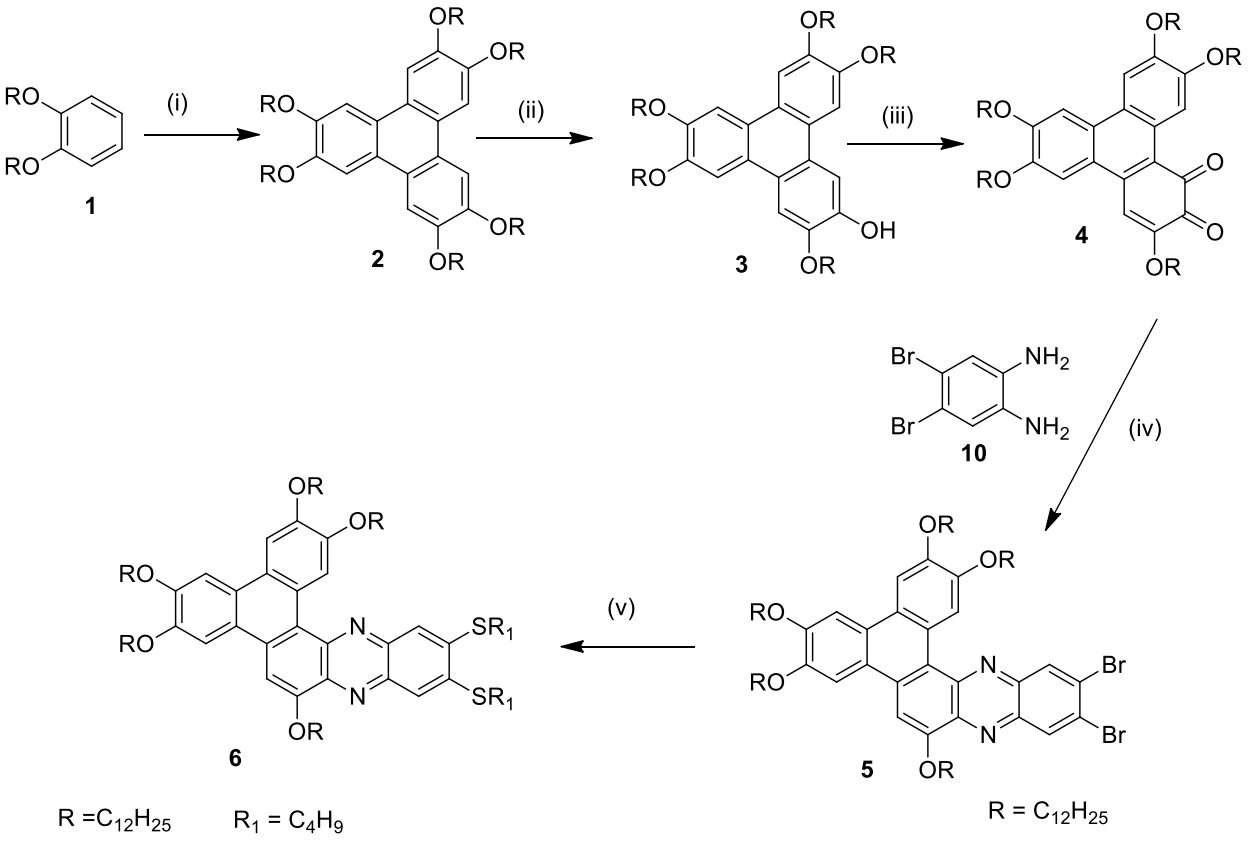
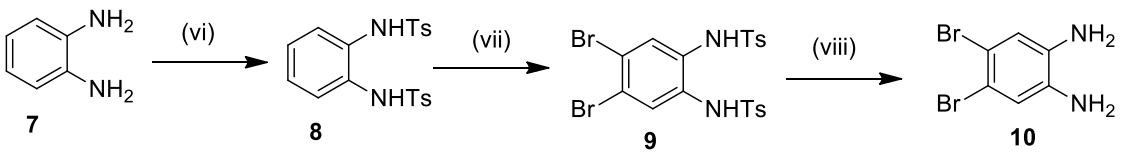
Synthesis of phenazine–fused triphenylene discotic liquid crystal

The synthesis of extended triphenylene fused mesogenic derivative as shown in **Scheme 1**.





Scheme 1. (i) $FeCl_3$, CH_2Cl_2, r.t, 30 min; (ii) catechol boron bromide, CH_2Cl_2, r.t, 24 h; (iii) CAN, CH_3CN, r.t, 30 min; (iv) CH_3COOH: toluene (7:3), reflux, 6 h; (v) alkanethiol, Cs_2CO_3, DMAC, reflux, 24 h; (vi) *p*-TosCl, pyridine, r.t, 24 h; (vii) Br_2, NaOAc, acetic acid, 110 ºC, 3 h; (viii) Con. H_2SO_4, 110 ºC, 15 min.

General procedure for the synthesis of final compound

The monohydroxytriphenylene **3** was synthesised by following reported procedure **[1]**. Oxidation of the 2-hydroxy-3,6,7,10,11-pentakis(alkyloxy) triphenylene **3** with ceric ammonium nitrate (CAN) gives 3,6,7,10,11-pentakis(alkyloxy)triphenylene-1,2-diones **4 [2]**. The intermediate 4,5-dibromobenzene-1,2-diamine **10** compound was synthesized following a reported procedure **[3]** and it was condensed with triphenylene-1,2-diquinone **4** in presence of glacial acetic acid in toluene (7:3) under reflux condition to afford intermediate 9,10-dibromo-2,3,6,14,15-pentaalkoxyphenanthro [9, 10-a]phenazine compounds **(5)**. Further, reaction of 1-butanethiol with intermediate mesogenic compound **5** in presence of cesium carbonate under reflux condition produces the desired extended phenazine based triphenylene mesogenic derivative **(6)**. All the intermediates and final compounds were purified by column chromatography, followed by recrystallization with appropriate solvent and well characterized using spectral and elemental analysis.

Reference

[1] S. Kumar, M. Manickam, Synthesis. 1998, 1119–1122.

[2] S. Kumar, M. Manickam, S. K. Varshney, D. S. S. Rao, S. K. Prasad, J. Mater. Chem. 2000, 10, 2483–2489

[3] J. Shao, J. Chang, C. Chi, Org. Biomol. Chem. 2012, 10, 7045–7052.

Figure S1. 3D crystal structure of CdS. It has been obtained using the refined parameters in VESTA software with ball-and-stick and polyhedron models of hexagonal phase.

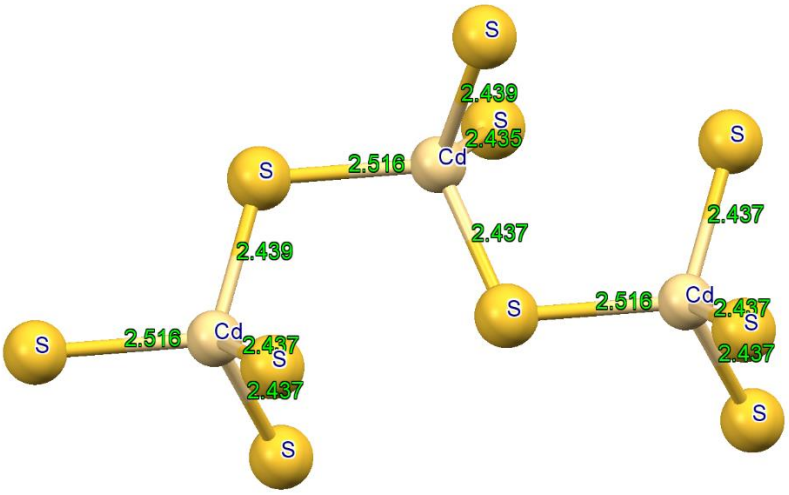


Figure S2. Average roughness profile of the PFT/CdS composite.

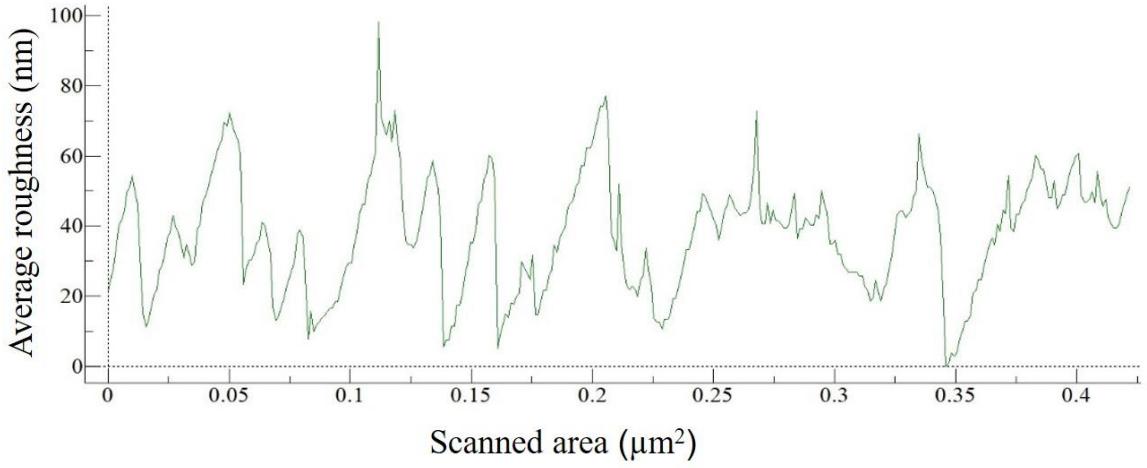


Figure S3. Thickness profilometric image of the ITO-PFTDLC/CdS-Au heterojunction.

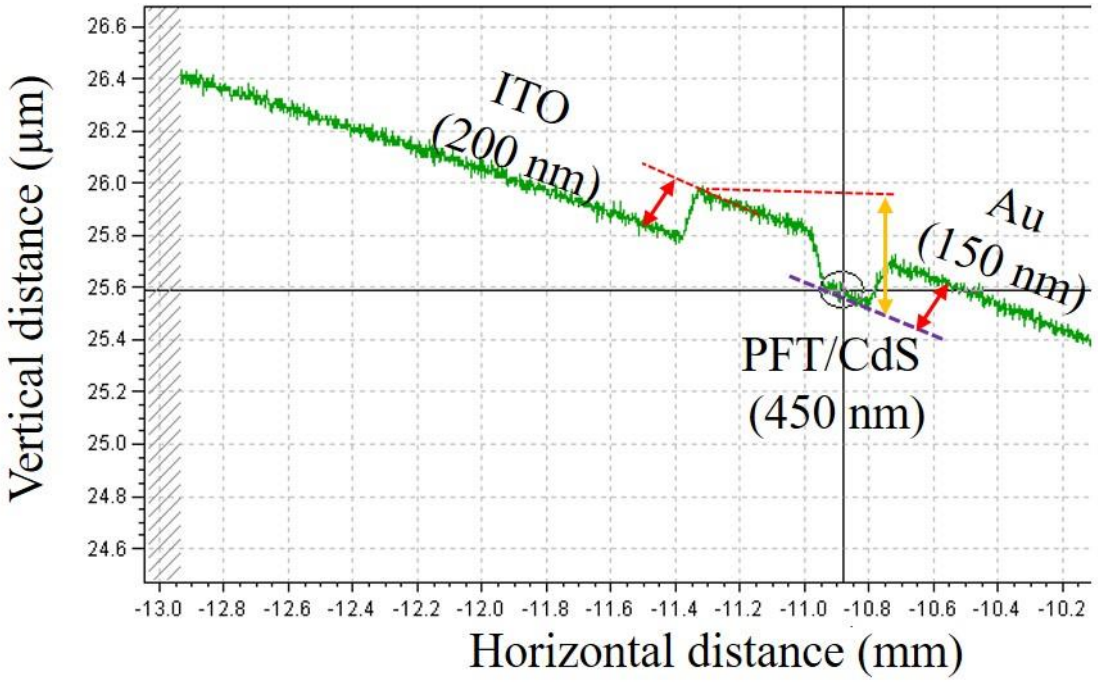


Figure S4. High resolution TEM image of CdS NWs.

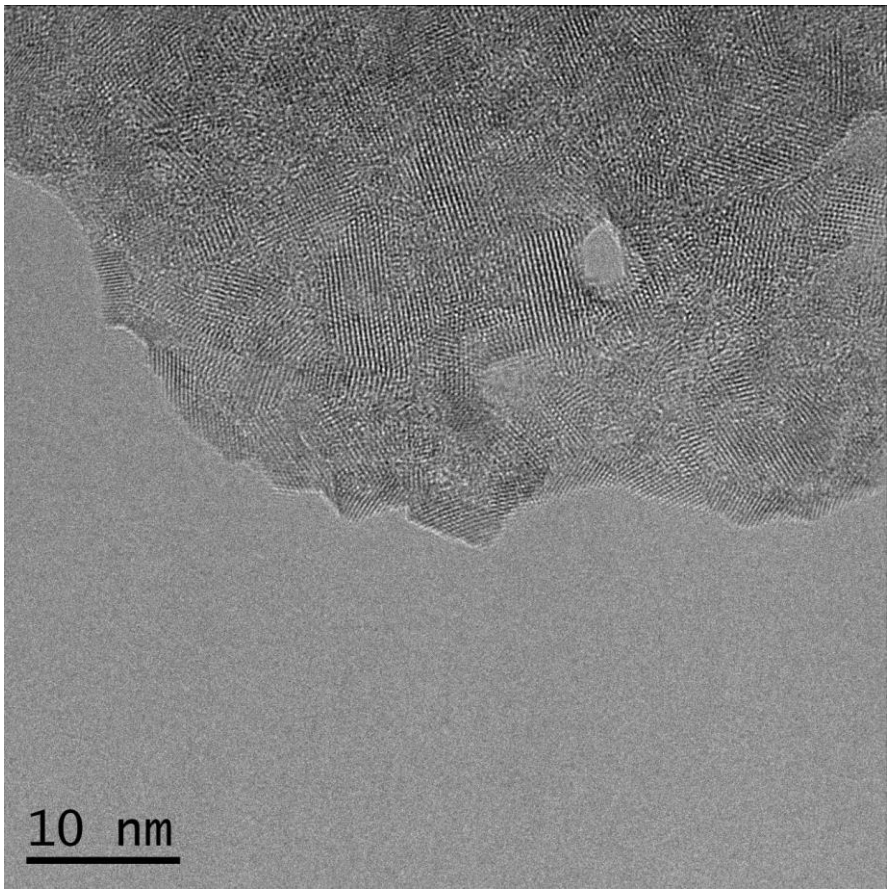


Table S1. X-ray data of the PFT DLC and PFT/CdS composite.

Compound	2θ (°)	d-spacing observed (calculated) Å	Phase/Lattice constant	Col_h parameter (r)	Miller indices	Alkyl-chain length (Å)	Core-Core separation (Å)	Intercolumnar distance (Å)
PFT DLC	3.59 6.22 7.19	24.58 (24.57) 14.19 (14.18) 12.28 (12.28)	Col_h a = 28.38	1 $1/\sqrt{3}$ 1/2	100 110 200	4.50	3.55	28.38
PFT/CdS composite	3.67 6.35 7.29	24.06 (24.05) 13.94 (13.89) 12.10 (12.02)	Col_h a = 27.78	1 $1/\sqrt{3}$ 1/2	100 110 200	4.47	3.50	27.78

Table S2. Details of transit time for the PFT DLC and PFT/CdS composite at 90 V.

Temperature (°C)	Transit time (PFT DLC) (sec)	Transit time (PFT/CdS composite) (sec)
70	0.000130175	1.40E-04
80	6.68805E-05	1.10E-04
90	4.06029E-05	8.44E-05
100	3.48631E-05	5.07E-05
110	2.90968E-05	4.26E-05
120	2.14839E-05	2.80E-05

Methods to calculate the hole mobility:

(I) Direct calculation method:

In this method, first we obtain a best transient photocurrent curve by examining it at various voltages; and we obtain the transit time (τ); then, the hole mobility (μ_h) is calculated using the formula; $\mu_h = d^2 / \tau.V$, where τ is the transit time obtained by photocurrent curves, V is the applied voltage and d is the thickness of ITO cell.

(II) Calculation via slope of transit time versus 1/V:

In this method, we first plot a curve between transit time and inverse of voltages (here we take several voltages) i.e. $\tau = \left(\frac{d^2}{\mu}\right)\left[\frac{1}{V}\right]$. In this relation the value of slope is equivalent to d^2/μ having intercept value equals to zero. Then mobility is calculated using the formula; $\mu = d^2 / slope$.