Supplementary Material (ESI) for Journal of Materials Chemistry

SUPPLEMENTARY INFORMATION

Synthesis and properties of fluorene or carbazole-based and dicyanovinyl-capped n-type organic semiconductors

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X-ray Diffraction Measurement. Crystal data of **FTCN**. The measurement was made on a Rigaku MM-007 diffractometer with Mo-Kα radiation (λ = 0.71073 Å) at room temperature. The structure was solved by direct methods and SHELXS-97, and refined by using SHELXL-97. Hydrogen atoms were located at the calculated positions. Absorption correction was applied using semi-empirical from equivalents. $C_{41}H_{36}N_4S_2$, M =648.86, crystal dimension 0.20 × 0.20 × 0.12 mm, monoclinic, space group $C2/c$, a = 33.557(10), b = 15.363(5), c = 13.991(5) Å, α = 90.00, β = 98.497(6), γ = 90.00°, V = 7134(4) Å^3, Z = 2, D_c = 1.208 g·cm^{-3}, μ = 0.183 mm^{-1}, θ range 1.23–26.41°, 20281 reflection collected, 7253 of which were independent (R_{int} = 0.1188), GOF = 1.046, 443 parameters, R_1 = 0.2015, wR_2 = 0.1292 for all reflections. CCDC 659317.

The original crystal structure exhibits that C33, C34 and C35 all have two diffractive sites respectively (Fig. S1), indicating that the odds of the carbon atoms in their two

sites are equal. In the full paper, we selected one situation to analyze its structure for clarity. Furthermore, seen from obtained X-ray crystallographic data, there are five diffractive sites found around the C32 atoms, indicating that the two H atoms combined with C32 are activated and oscillatory surrounding the C32 atom. The selected two sites happened in the positions far from C32 that bring the deviations, so the two H atoms are not showed in the original structural Fig. but marked in the full paper.

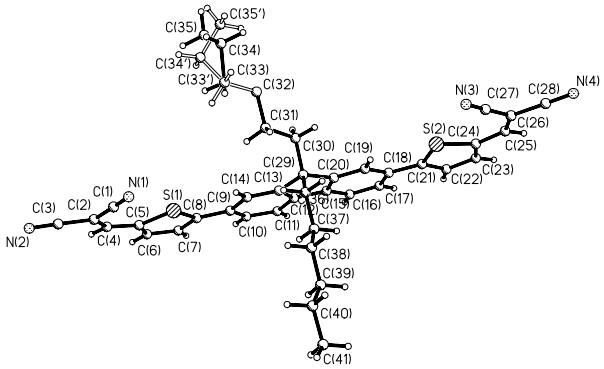

Fig. S1. The original crystal structure of **FTCN**.

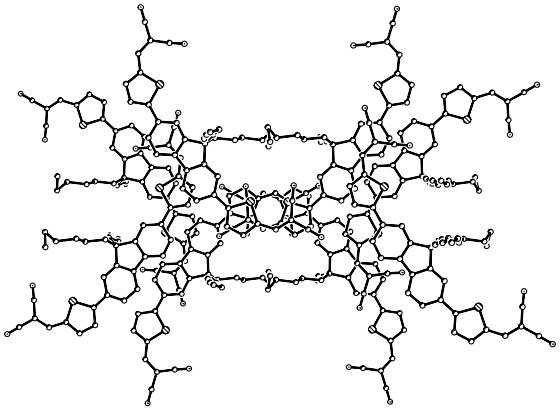

Fig. S2. View down the c-axis in crystals of **FTCN**, hydrogen atoms removed for clarity.

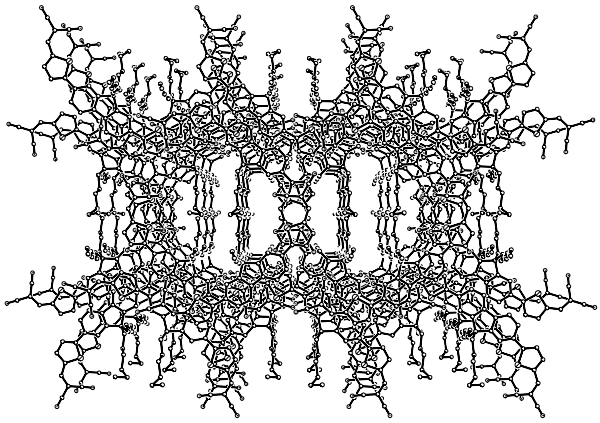

Fig. S3. Crystal packing of **FTCN** down the c-axis, hydrogen atoms removed for clarity.

Optical and Electrochemical Measurements. The UV-vis absorption spectra were measured using a Hitachi Model U-3010 Spectrometer. Emission spectra were recorded on Hitachi F-4500 fluorescence spectrometer. Cyclic voltammetric measurements were carried out in a conventional three-electrode cell using Pt button working electrodes of 2 mm diameter, a platinum wire counter electrode, and a Ag/AgCl reference electrode on a computer-controlled CHI660C instruments at R. T.

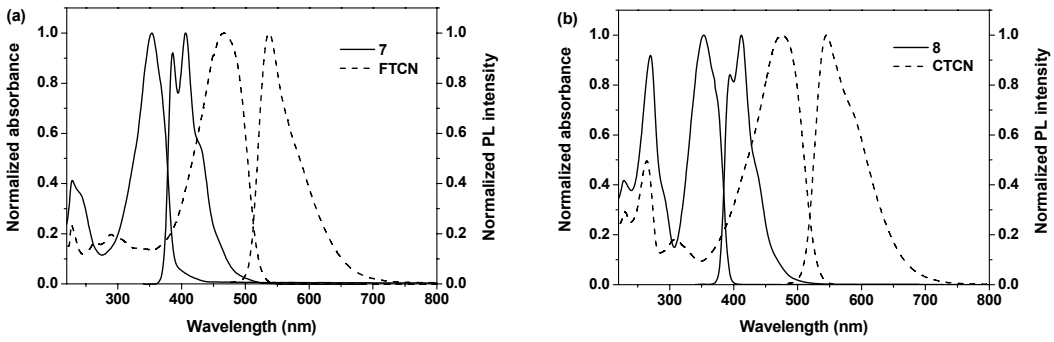

Fig. S4. Optical properties of compounds measured in CH_2Cl_2 solution. (a) Compounds **7** and **FTCN**. (b) Compounds **8** and **CTCN**.

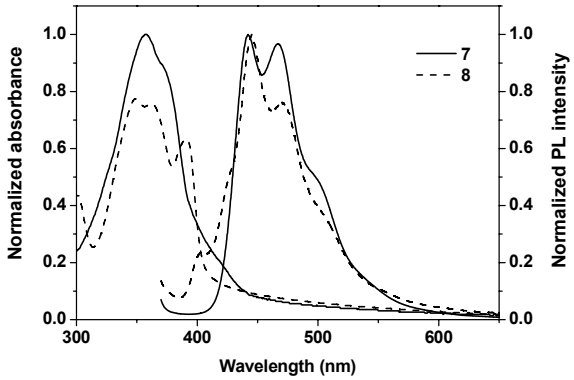

Fig. S5. Optical properties for films of molecules **7** and **8**.

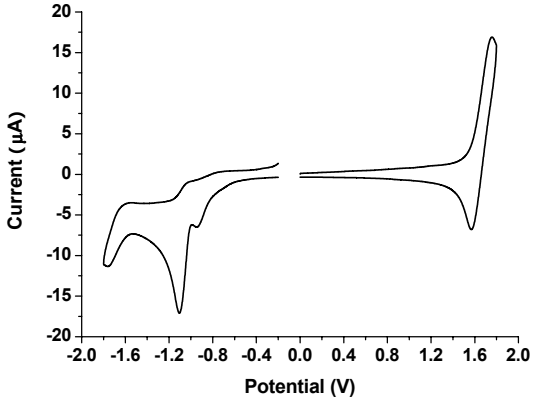

Fig. S6. Cyclic voltammogram of **FBCN** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV/s).

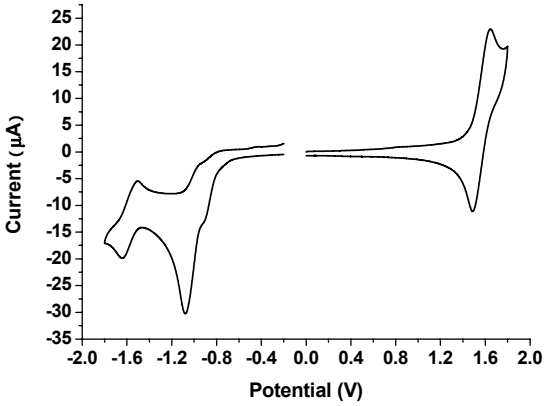

Fig. S7. Cyclic voltammogram of **FTCN** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100

mV/s).

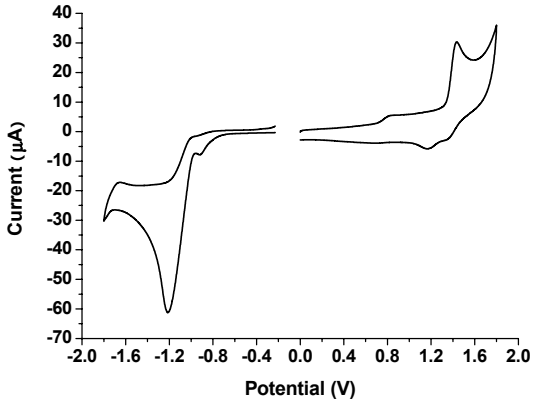

Fig. S8. Cyclic voltammogram of **CBCN** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV/s).

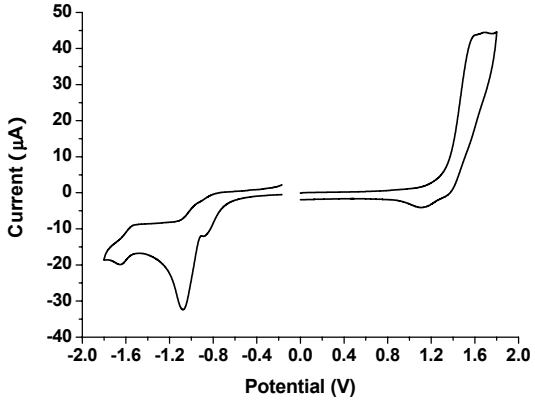

Fig. S9. Cyclic voltammogram of **CTCN** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV/s).

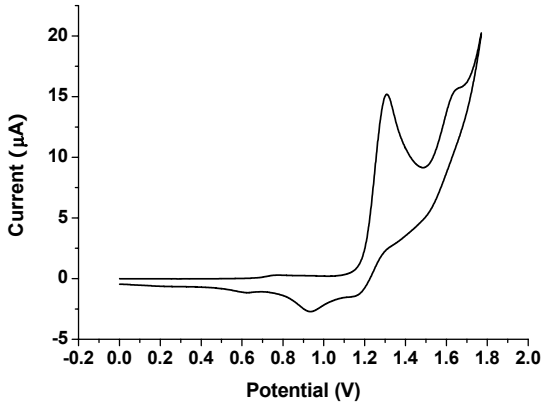

Fig. S10. Cyclic voltammogram of **7** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV/s).

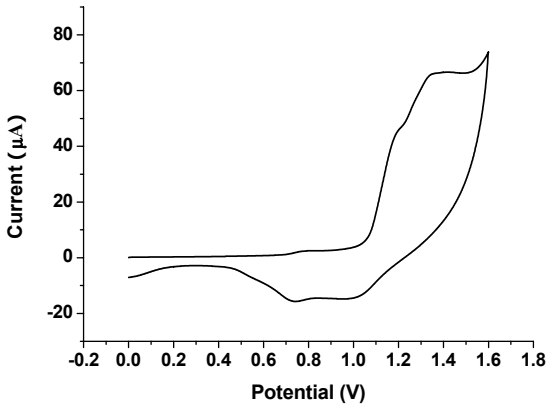

Fig. S11. Cyclic voltammogram of **8** (0.1 M n-Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV/s).