Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Efficiency enhancement in indacenodithiophene and thieno[3,4-*c*]pyrrole-4,6-dione backboned photovoltaic polymer with extended thieno[3,2-*b*]thiophene π-bridge†

Huilin Zheng,[a, b]† Jiuxing Wang,[b, d]† Weiye Chen,[a, b] Chuantao Gu,[b, d] Junzhen, Ren,[a, b] Meng Qiu,[b] Renqiang Yang,*[b] Mingliang Sun*[a]

a. Institute of Materials Science and Engineering, Ocean University of China, Qingdao 266100, China. E-mail: mlsun@ouc.edu.cn

b. CAS key Laboratory of Bio-based Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy Science, Qingdao 266101, China. E-mail: yangrq@qibebt.ac.cn

c. State Key Laboratory of Luminescent Materials and Devices , South China University of Technology, Guangzhou 510640, China

d. University of Chinese Academy of Sciences, Beijing 100049, China

† These authors contributed equally to this work.

1. Materials

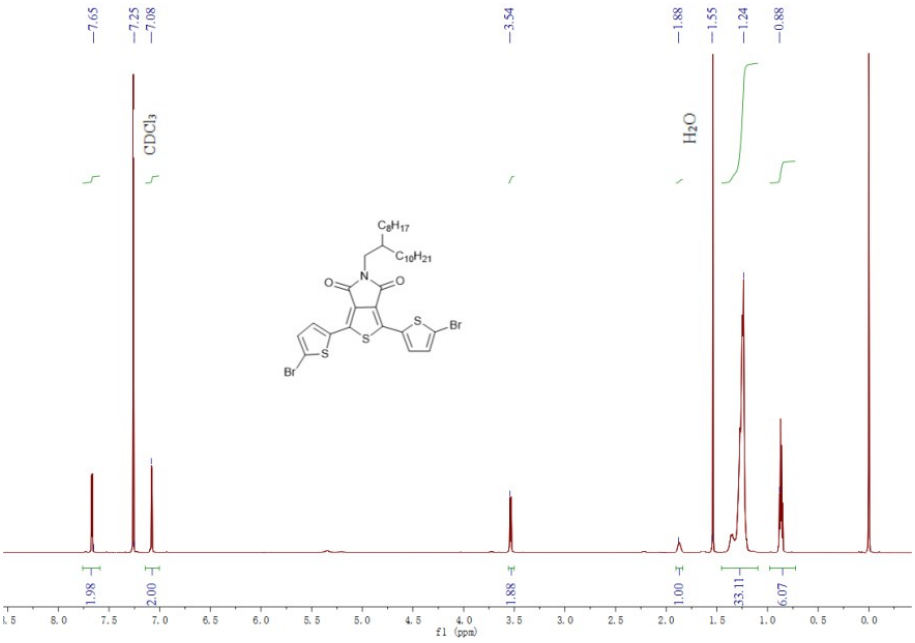

Fig. S1 ^{1}H NMR spectra of momomer T-TPD.

T-TPD: ^{1}H NMR (600 MHZ, $CDCl_3$, TMS), δ (ppm): 7.65 (d, J = 4.0 Hz, 2H), 7.08 (d, J = 4.0 Hz, 2H), 3.54 (d, J = 7.3 Hz, 2H), 1.87 (s, 1H), 1.45-1.09 (m, 32H), 0.88 (t, J = 6.0 Hz, 6H).

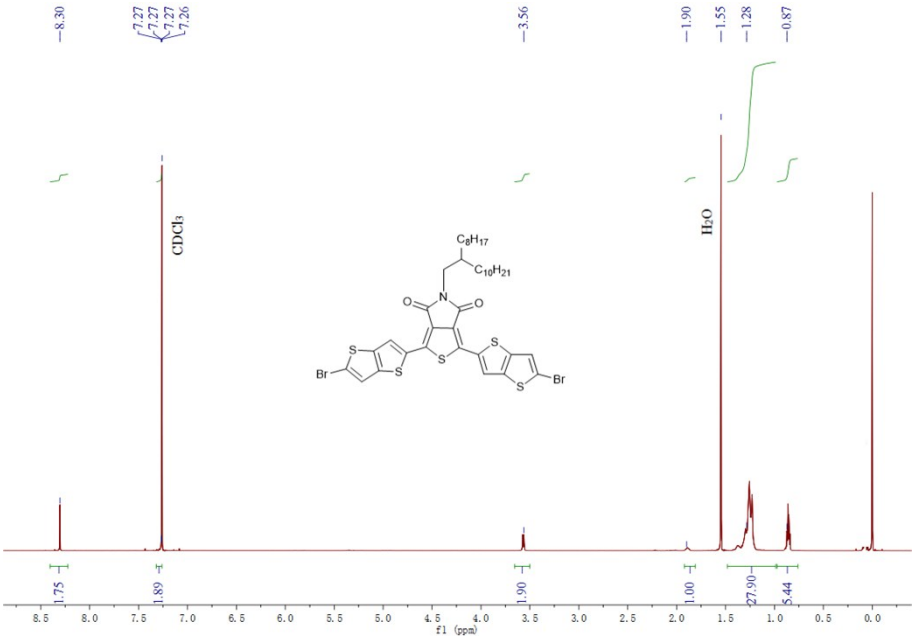

Fig. S2 [1]H NMR spectra of momomer TT-TPD.

TT-TPD: [1]H NMR (600 MHZ, $CDCl_3$, TMS), δ (ppm): 8.30 (s, 2H), 7.27 (s, 2H), 3.57 (d, J = 7.3 Hz, 2H), 1.89 (s, 1H), 1.45-1.02 (m, 32H), 0.86 (t, J = 6.8 Hz, 6H).

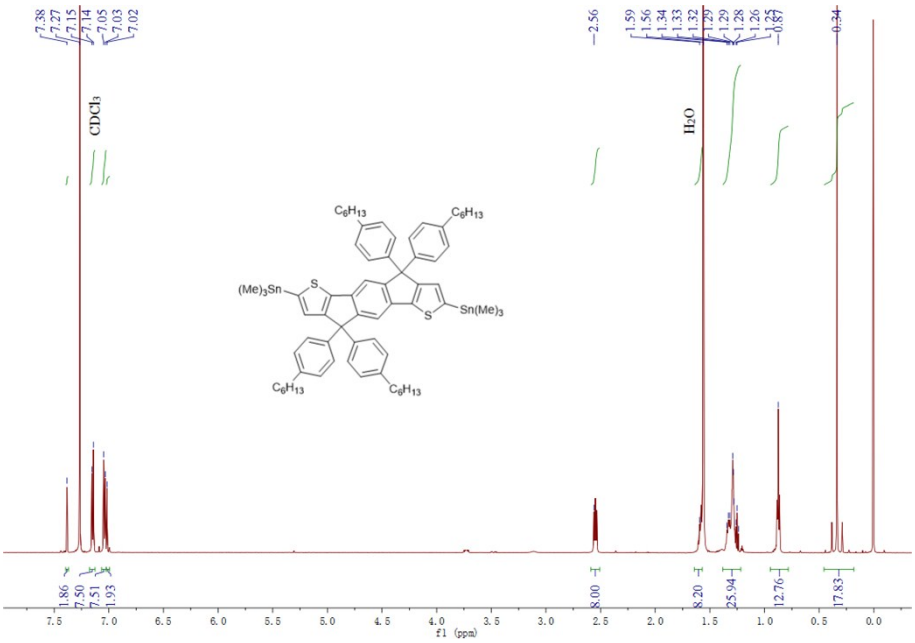

Fig. S3 [1]H NMR spectra of momomer IDT-di-Tin.

IDT-di-Tin: [1]H NMR (600 MHZ, $CDCl_3$, TMS), δ (ppm): 7.38 (s, 2H), 7.15 (d, J = 8.2 Hz, 8H), 7.04 (d, J = 8.2 Hz, 8H), 7.02 (s, 2H), 2.55 (t, J = 7.9 Hz, 8H), 1.64-1.57 (m, 8H), 1.36-1.22 (m, 24H), 0.87 (t, J = 6.9 Hz, 12H), 0.34 (s, 18H).

2. Instrument

^{1}H NMR spectra were recorded using a Bruker DRX-600 (600 MHz) spectrometer in $CDCl_3$ with tetramethylsilane (TMS) as internal standard and in ambient conditions. Elemental analysis data was recorded on a Vario EI Cube elemental analyzer. The molecular weight of the polymer was measured by gel permeation chromatography (GPC), and polystyrene was used as an standard, THF as the eluent. Thermogravimetric analysis (TGA) measurements were performed by a STA-409 at a heating rate of 10 °C min^{-1} under nitrogen atmosphere. X-ray diffraction (XRD) spectra were recorded on a Bruker D8 Advance Spectra. Ultraviolet-visible (UV-vis) absorption spectra were recorded using a Hitachi U-4100 spectrophotometer. Cyclic voltammetry (CV) was performed on a CHI 660D electrochemical workstation with a three-electrode system consisting of a platinum disk working electrode (2.0 mm in diameter), a saturated calomel reference electrode (SCE) and a platinum wire counter electrode in a solution of 0.1 M tetrabutylammonium phosphorus hexafluoride (Bu_4NPF_6) in acetonitrile at a scan rate of 50 mV s^{-1}. Polymer thin films were deposited from DCB solution onto the platinum working electrodes and dried under nitrogen prior to measurement. The redox potential of the ferrocene/ferrocenium (Fc/Fc^+) internal reference is 0.39 V vs. SCE. The space-charge-limited current (SCLC) measurements were carried out using an HZ-5000 electrochemical analyzer. Surface roughness and morphology of thin films were characterized by atomic force microscopy (AFM) on an Agilent 5400 and transmission electron microscope by HITACHI H-7650.

3. Thermal gravity analysis (TGA)

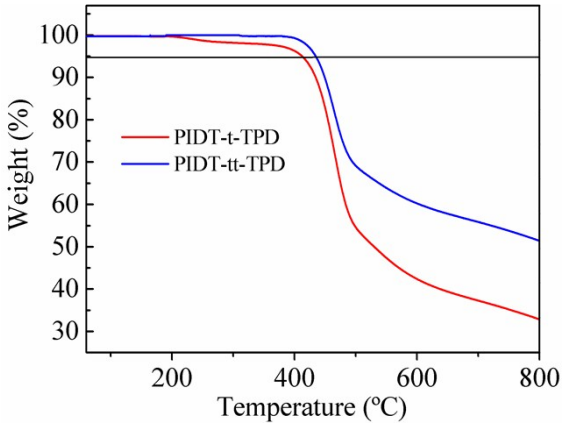

Fig. S4 TGA plot of PIDT-t-TPD and PIDT-tt-TPD under nitrogen atmosphere.

4. X-ray diffraction

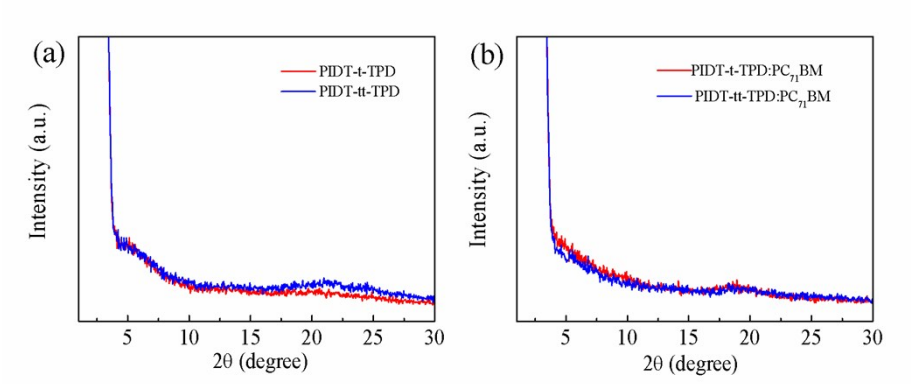

Fig. S5 XRD patterns of pure polymers (a) and polymer/$PC_{71}BM$ blend films (b).

5. Optical properties

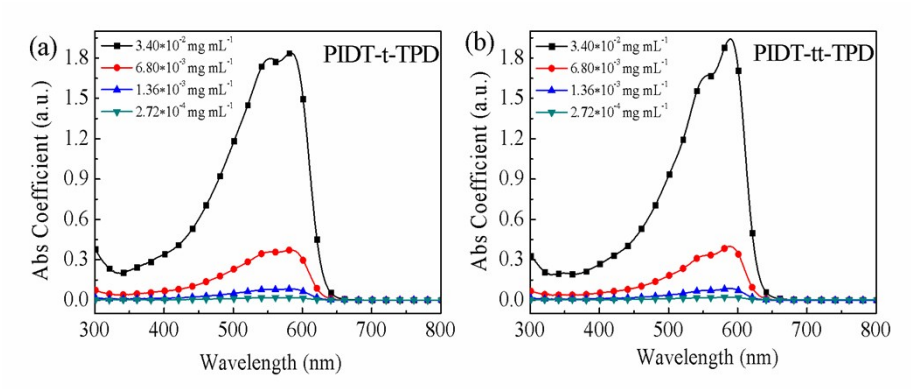

Figure S6. UV-vis absorption spectra of PIDT-t-TPD and PIDT-tt-TPD dissolved in DCB at various concentrations.

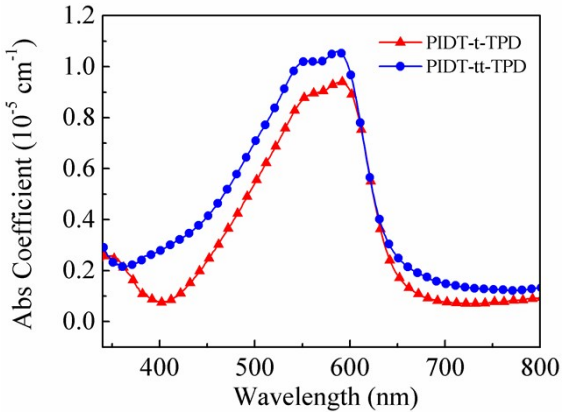

Fig. S7 Extinction coefficients of the polymer films.

6. Hole mobility

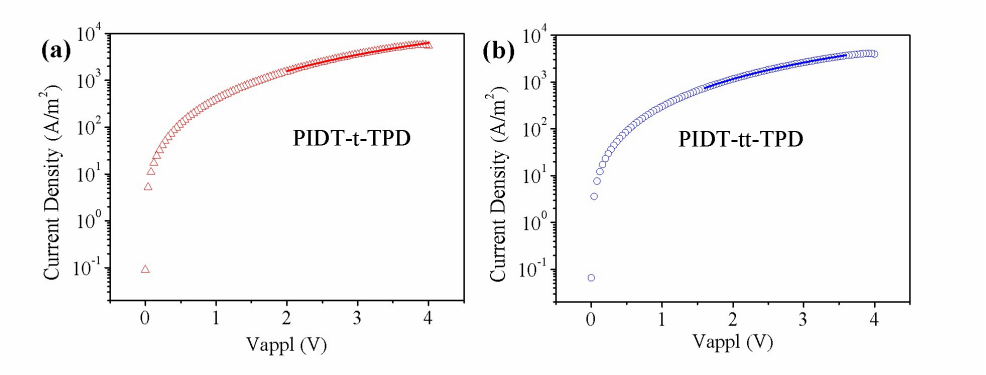

Fig. S8 Current density-voltage (*J-V*) curves for PIDT-t-TPD:$PC_{71}BM$ based device (a) and PIDT-tt-TPD: $PC_{71}BM$ based device (b) (the symbols are experimental data for transport of hole, and the solid line is fitted according to the space-charge-limited-current model). The configuration of the devices is ITO/PEDOT:PSS/polymer:$PC_{71}BM$/MoO_3/Al.