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Supporting information

Extended π-Conjugated Area of Electron-Donating Units in D-A Structured Polymers towards High-Mobility Field-Effect Transistors and Highly Efficient Polymer Solar Cells

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1. Experimental section

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 300 spectrometer with tetramethylsilane (TMS) as the internal reference. Molecular weights of the polymers were obtained on a Waters GPC 2410 using a calibration curve of polystyrene standards, with tetrahydrofuran as the eluent, or on a PL GPC 220 (Polymer Laboratories) at 150 °C using a calibration curve of polystyrene standards, with 1,2,4-trichlorobenezene as the eluent. Elemental analyses were performed on a Vario EL elemental analysis instrument (Elementar Co.). Thermogravimetric (TGA) measurements were carried out with a NETZSCH (TG209F3) apparatus at a heating rate of 20 °C /min under a nitrogen atmosphere. Differential scanning calorimetry (DSC) analysis was performed on a NETZSCH (DSC200F3) apparatus at a heating or cooling rate of 10 °C /min under a nitrogen atmosphere. UV-vis absorption spectra were recorded on a SHIMADZU UV-3600 spectrophotometer. Cyclic voltammetry (CV) was carried out on a CHI660A electrochemical workstation with platinum electrodes at a scan rate of 50 mV s^{-1} against an

Ag/Ag^+ reference electrode with nitrogen-saturated solution of 0.1 M tetrabutylammonium hexafluorophosphate(Bu_4NPF_6) in acetonitrile (CH_3CN). Potentials were referenced to the ferrocenium/ferrocene couple by using ferrocene as an internal standard. The deposition of a copolymer on the electrode was done by the evaporation of a chlorobenzene solution. Tapping-mode atomic force microscopy (AFM) images were obtained using a NanoScope NS3A system (Digital Instrument).

FET fabrication and characterization

To measure the hole mobilities of the polymer, FETs were fabricated in a top contact geometry using silver as the source and drain electrode. Highly n-doped silicon and thermally grown silicon dioxide (300 nm) were used as the back gate and gate dielectric, respectively. Octyltrichlorosilane (OTS) was then used for surface modification of the gate dielectric layer. The copolymer film (50 nm) was spin-coated on OTS treated substrates from a dichlorobenzene solution. Then silver film (60 nm) was deposited under vacuum as the source and drain electrodes. The width to length ratio (W/L) of the FET devices is 100/1. The FETs characterizations were performed in the atmosphere by using a probe station and a semiconductor parameter analyzer (Agilent 4155C). Then field-effect mobility was calculated from the standard equation for saturation region in metal–dioxide–semiconductor field effect transistors: $I_{DS}=(W/2L)\mu C_i(V_G - V_{th})^2$, where I_{DS} is the drain-source current, μ is the field-effect mobility, W and L are the channel width and length, C_i is the capacitance per unit area of the dielectric layer (C_i = 10.4 nF cm^{-2}), V_G is the gate voltage, and V_{th} is the threshold voltage.

PSC fabrication and characterization

Patterned indium tin oxide (ITO)-coated glass with a sheet resistance of 15–20 ohm/square were cleaned by a surfactant scrub, then underwent a wet-cleaning process inside an ultrasonic bath, beginning with deionized water, followed by acetone and isopropanol. A methanol solution of PFN was spin-coated on the top of the ITO substrate and dried at 100

°C for 10 min to form a thin interlayer of 5 nm.[1] The active layers were deposited on top of the PFN interlayer, by casting from dichlorobenzene solutions, and drying at 60 °C for 10 min. The thickness of an active layer was verified by a surface profilometer (Tencor, Alpha-500). At a base pressure of 3×10^{-4} Pa, a 10 nm MoO_3 was thermally evaporated at an evaporation rate of 0.1 Å/s. Finally, a 100 nm aluminium layer was evaporated with a shadow mask. The overlapping area between the cathode and anode defined a pixel size of 0.16 cm^2. The thickness values of the evaporated MoO_3 and Al were monitored by a quartz crystal thickness/ratio monitor (Model: STM-100/MF, Sycon). All the fabrication processes were carried out inside a controlled atmosphere of nitrogen dry-box (Vacuum Atmosphere Co.) containing less than 10 ppm oxygen and moisture. The power conversion efficiencies of the resulting polymer solar cells were measured under 1 sun, AM 1.5G (air mass 1.5 global) spectrum from a solar simulator (Oriel model 91192) (100 mW/cm^2). The current density–voltage (J–V) characteristics were recorded with a Keithley 2410 source unit.

References

1. Z. C. He, C. Zhang, X. F. Xu, L. J. Zhang, L. Huang, J. W. Chen, H. Wu, Y. Cao, *Adv. Mater.* **2011**, *23*, 3086

Supplementary figures

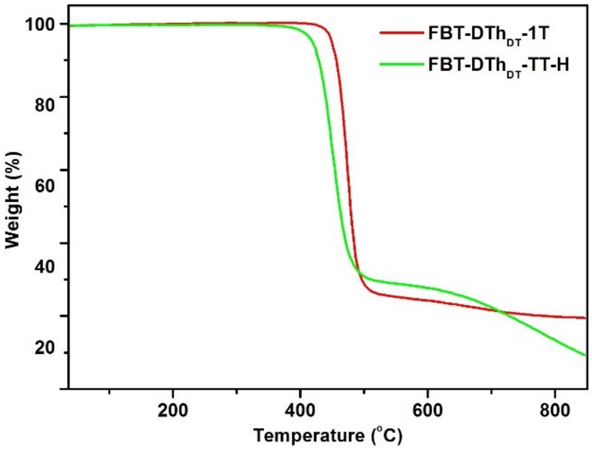

Figure S1. Thermogravimetric analysis of FBT-DTh$_{DT}$-1T and FBT-DTh$_{DT}$-TT-H at a heating rate of 20 °C/min under a nitrogen atmosphere.

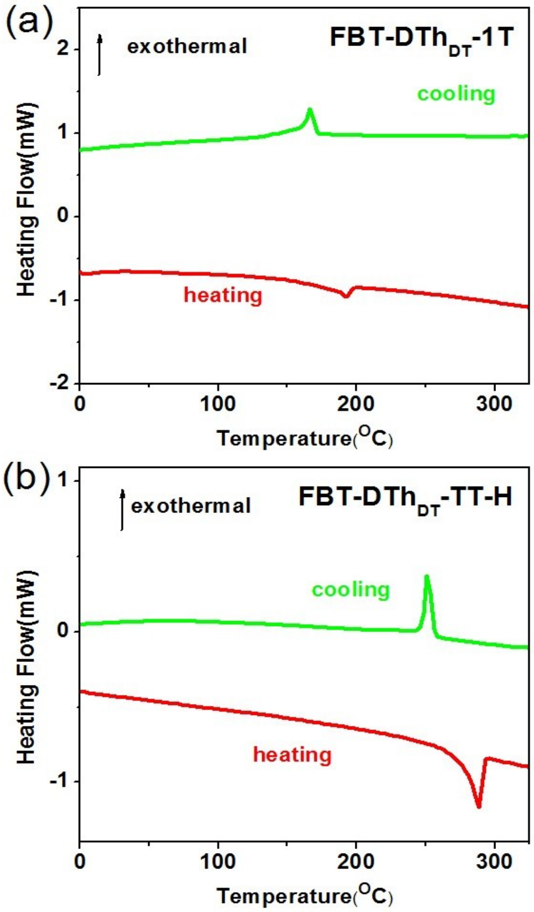

Figure S2. Differential scanning calorimetry thermograms of FBT-DTh$_{DT}$-1T (a) and FBT-DTh$_{DT}$-TT-H (b) at a heating or cooling rate of 10 °C /min under a nitrogen atmosphere.

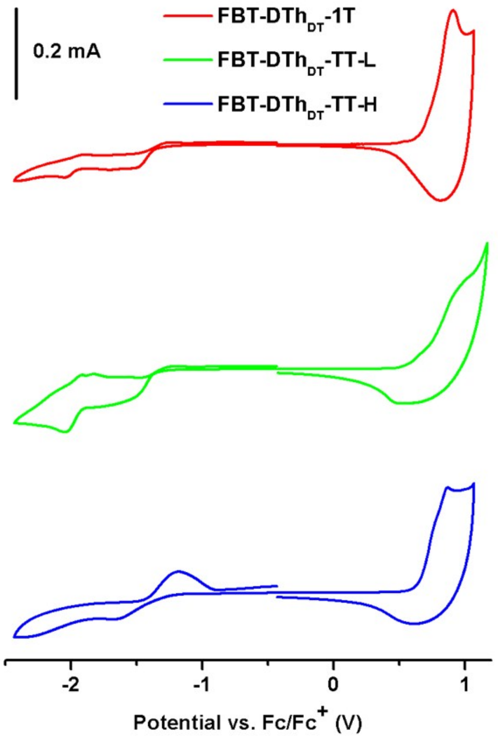

Figure S3. Cyclic voltammogram of polymers with an Ag/Ag$^+$ electrode as the reference electrode and an energy level of ferrocene of −4.80 eV as the internal standard.

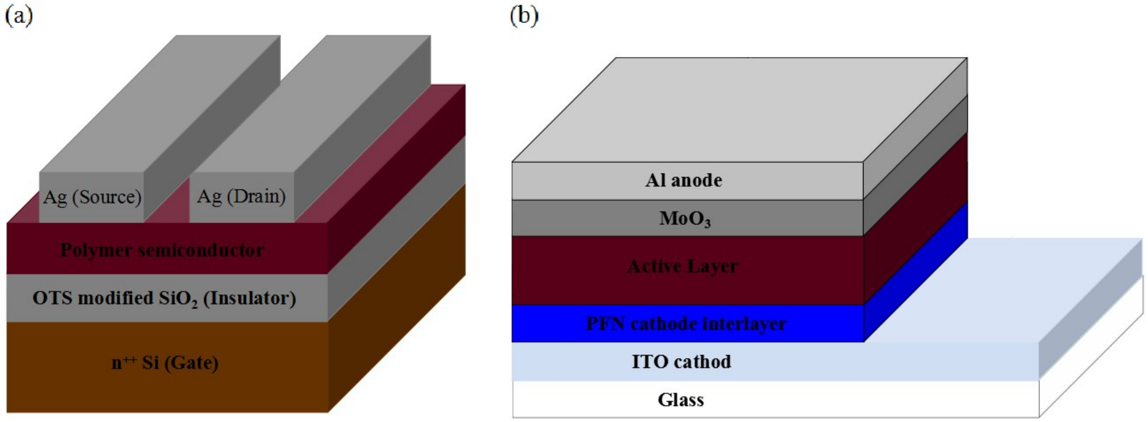

Figure S4. Device configurations of (a) the top-contact field effect transistors and (b) the inverted polymer solar cells.

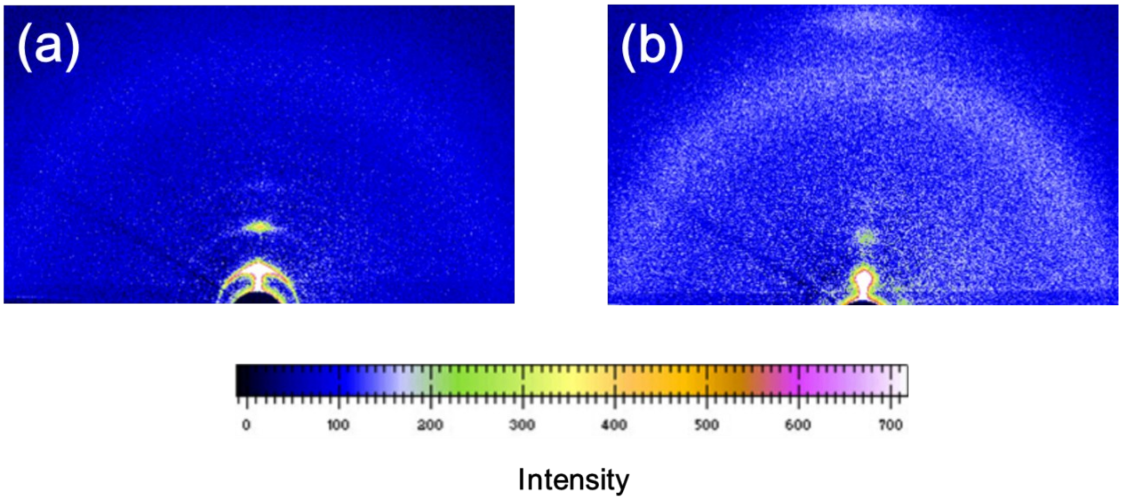

Figure S5. Grazing incidence wide-angle X-ray diffraction (GIXD) patterns of (a) FBT-DTh$_{DT}$-TT-L film and (b) FBT-DTh$_{DT}$-TT-H film.

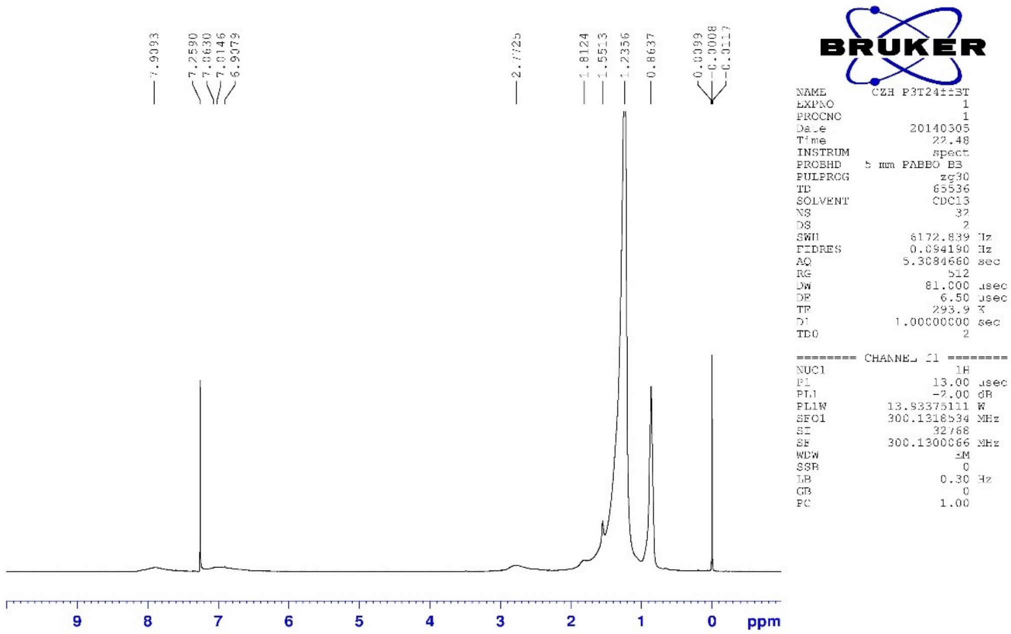

Figure S6. ^{1}H NMR of polymer **FBT-DTh$_{\mathbf{DT}}$-1T**.

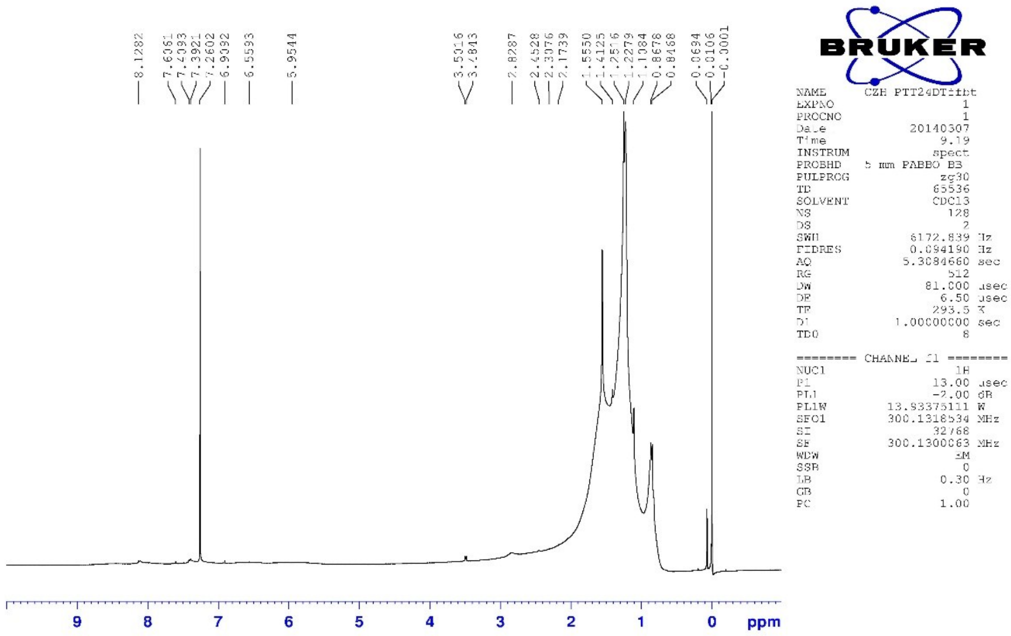

Figure S7. ^{1}H NMR of polymer **FBT-DTh$_{\mathbf{DT}}$-TT-L**.