Charge Generation and Transport in Efficient Organic BHJ Solar Cells with Non-fullerene Acceptor

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SUPPLIMENTARY INFO:

Device fabrication:

Inverted devices were fabricated on patterned ITO-coated glass substrate. The ITO substrates were cleaned with RCA treatment (a mixture of hydrogen peroxide (H2O2), ammonium hydroxide (NH4OH) and water (1:1:5 by volume) at 80 °C for 15 minutes) to make substrate hydrophilic. The zinc acetate dihydrate (314 mg), 2-methoxyethanol (3.14 mL), and ethanolamine (86 µL) was mixed and stirred vigorously for 2 h at 60 °C in air. The precursor is now spin coated at 2000 rpm on to cleaned ITO substrates to get a smooth ZnO films. Crystalline ZnO films were obtained by subsequent annealing of substrate at 250 °C for 30 min in air. The blends of different weight ratio of PBDTTT-CT:TP is mixed in anhydrous chlorobenzene with blend concentration of 12 mg/mL. These blend solutions were spin coated on to ZnO substrate inside the glove box at 1000 rpm. The Hole transport layer MoOx (≈11 nm) and Ag (≈100 nm) was deposited by shadow mask method through physical vapor deposition at a base pressure of 10^{-6} mbar.

For SCLC measurements, the electron only device is fabricated on to ZnO coated ITO substrate working as electron extracting and Al as electron injecting electrode. The hole only device were fabricated on to MoO_x coated ITO substrate working as hole injecting and MoO_x/Ag as hole

extracting electrode. All the films were coated at 100 rpm with blend concentration of 12 mg/ml. The thicknesses of active layer were measured using Dektak profilometer exhibiting thickness in the range of 1.5 - 2.5 µm.

Internal quantum efficiency measurements:

The internal quantum efficiency $\eta_{IQE}(\lambda)$ (Ref 1) was obtained from the following equation:

$$\eta_{IQE}(\lambda) = \frac{\eta_{EQE}(\lambda)}{abs(\lambda)}$$

Where, $\eta_{EQE}(\lambda)$ is the external quantum efficiency and $abs(\lambda)$ is the percentage absorbance. The overall $abs(\lambda)$ absorbance (%) of the devices is calculated from the transmission mode spectra of the films coated on ZnO-ITO substrates. It was made certain that these films were identical (thickness) to films used for the active devices.

Reference:

1) Jinsong Huang and Yang Yang, Origin of photomultiplication in C60 based devices, Applied Physics Letters, 91, 203505, 2007.
2) Gilles Dennler, Karen Forberich, Markus C. Scharber, Christoph J. Brabec, Igor Tomiš, Kurt Hingerl, and Thomas Fromherz, Angle dependence of external and internal quantum efficiencies in bulk-heterojunction organic solar cells, Journal of Applied Physics, 102, 054516, 2007.

Excitation density dependence:

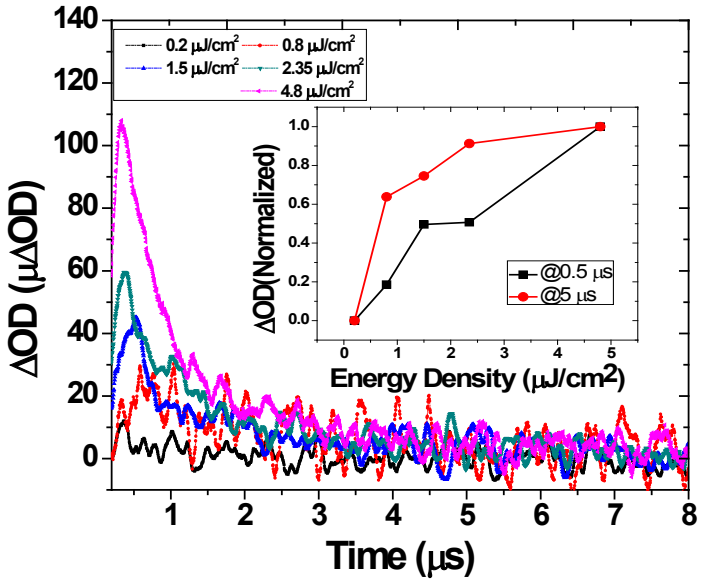

Fig. S1 Excitation density dependence with ΔOD(t)(all transient are probed at 920 nm excited at 700 nm), Inset shows the normalized ΔOD(t) vs excitation density at 0.5 μs and 5 μs.

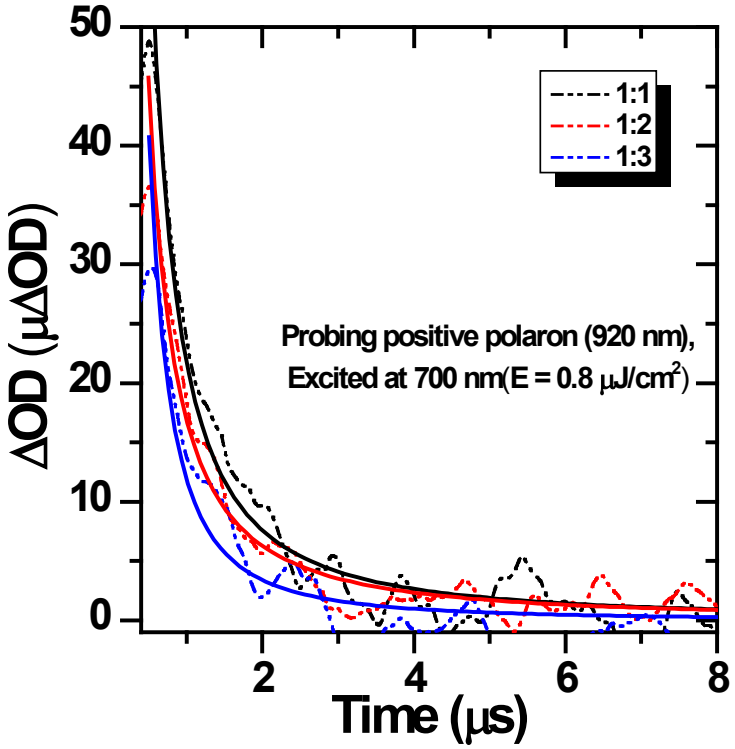

Fig. S2 Concentration dependence on the TAS.

Comparison of transient signal with different acceptors:

Blend (1:1 wt/wt)	*α*	*A*
PBDTTT-CT:PCBM	1.07	7.27×10^{-12}
PBDTTT-CT:TBP	1.13	2.68×10^{-12}
PBDTTT-CT:PIP	0.28	1.24×10^{-7}

Table 1: *Parameters used for Power law decay fit of different blends transient decay dynamics.*

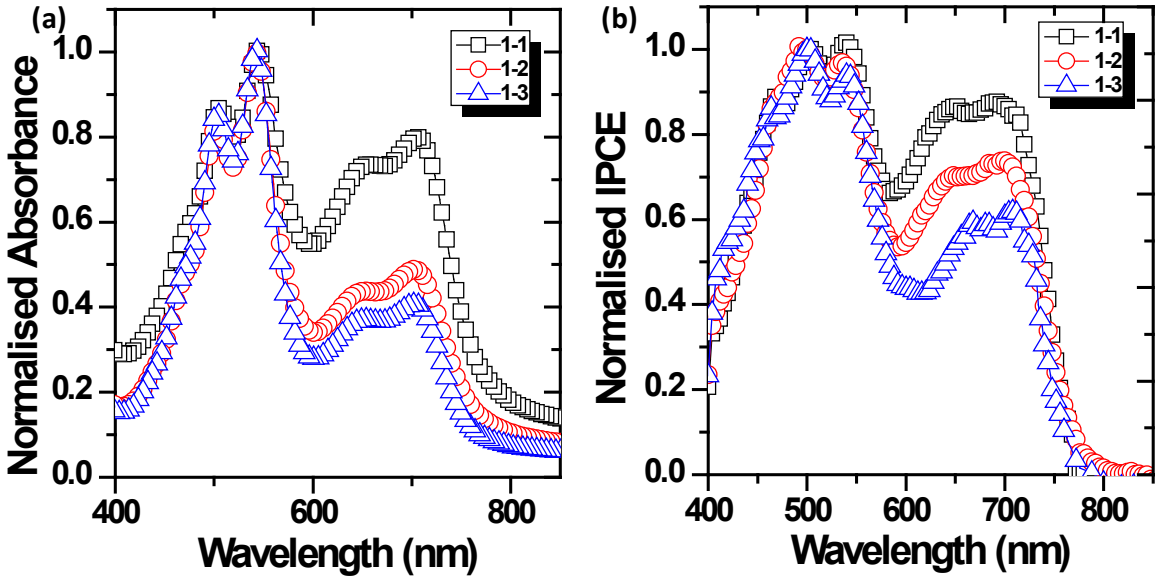

Fig. S3 (a) Normalised absorption of blends of 1:1, 1:2 and 1:3 with respect to their maxima. All films were spun coated from 12 mg/ml solution of blend in chlorobenzene at 1000 rpm. (b) normalized IPCE with respect to IPCE at λ = 500 nm follows a consistent behavior absorption of blends and indicates increased contribution from TP excitons in charge generation.

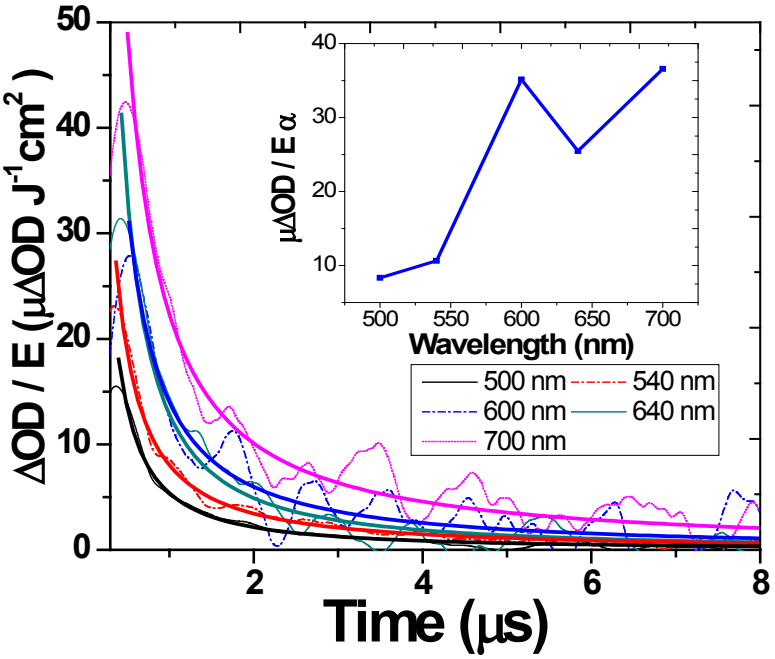

Fig. S4 Transient absorption of PBDTTT-CT:TBP (1:1) probed at 920 nm and pulsing at different wavelength. Inset shows the efficiency of charge generation at different wavelength.

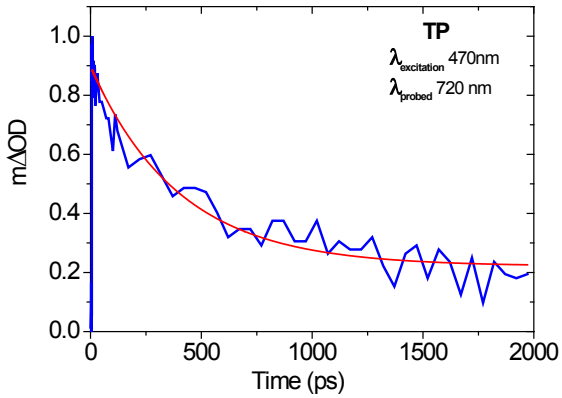

Fig. S5 Transient decay dynamics of Pristine TP excited at 470 nm and probed at 720 nm. The red curve is an exponential fit of the decay .

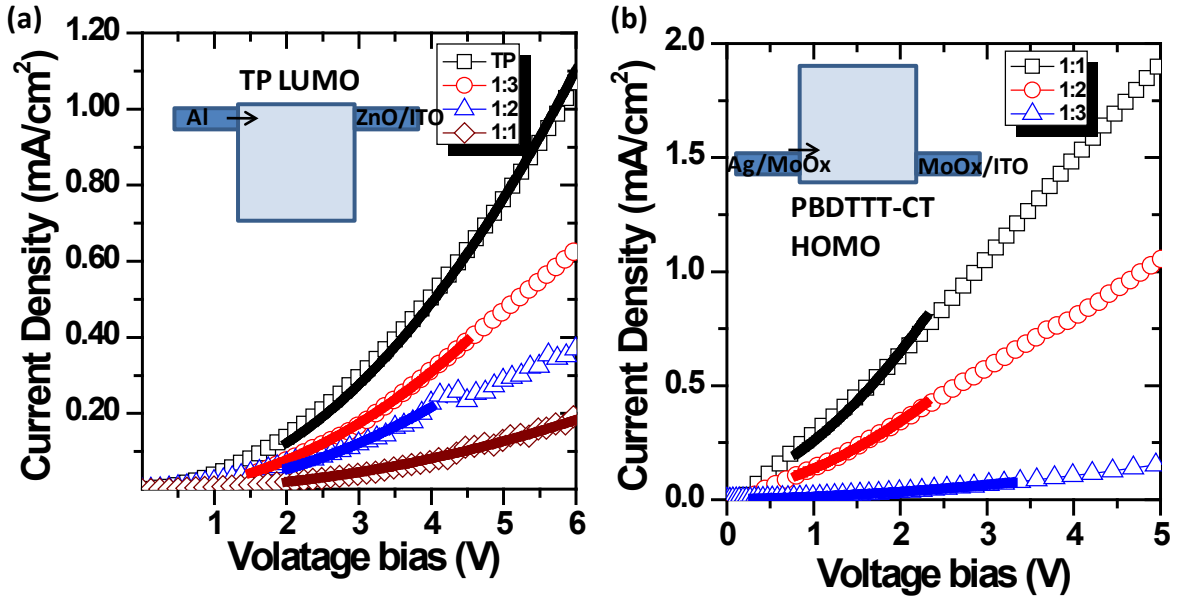

Fig S6 SCLC measurement showing the *J- V* curves for electron-only(a) and hole-only(b) devices consisting of different TP compositional ratio in the blend. The applied bias voltage is corrected for the built-in potential (V_{bi}) so that $V=V_{\text{applied}}-V_{\text{bi}}$.