

Supporting information

Efficient Ternary Bulk Heterojunction Organic Solar Cells Using A Low-cost Nonfullerene Acceptor

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Device Fabrication and Characterization

The solution processed BHJ PSCs (binary as well as ternary active layers) were fabricated with a conventional device structure of indium tin oxide (ITO)/PEDOT:PSS (40 nm)/active layer/ PFN(20 nm) /Al (50 nm). Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) and Poly[(9,9-bis(3-(N,N-dimethylamino)propyl)-2,7-fluorene)-alt-2,7-(9,9-dioctylfluorene)] (PFN) were used as hole transport layer (HTL) and electron transport layer, respectively. The fabrication details are as follows: ITO coated glass substrates were cleaned before the device fabrication in acetone, detergent, deionized water, isopropyl alcohol in ultrasonic bath, sequentially, and then dried in a vacuum oven. A thin film of PEDOT:PSS was spin-casted onto the ITO coated glass substrates at 3000 rpm for 30 min and then thermally annealed at 120° C for 30 min. The binary and ternary active layers were prepared from the donor **P** and acceptors (PC₇₁BM or **Cz-IC**) *via* varying the weight ratio between donor and acceptor with an overall concentration of 16 mg/mL. Then, the solution was spin casted on top of the PEDOT:PSS film and then dried. In order to prepare the ternary active layers, the weight ratio between two acceptors (PC₇₁BM and **Cz-IC**) was varied keeping the concentration of donor **P** constant. After the solvent vapor annealing (SVA) exposure, the films were removed from the petri dish and were allowed to dry at room temperature for 1 min. The thickness of the films was about 90 ± 5 nm. A thin film of PFN in methanol solution (0.1 mg/mL) was spin coated on top of the active layer to form the ETL and then dried. Finally, a

thin film of aluminium (Al) was thermally deposited on top of PFN at pressure less than 1×10^{-5} torr with a shadow mask on top of the electrode. The effective area of the devices was 0.16 cm^2 . The power conversion efficiencies of the devices were determined from the current-voltage characteristics measured by Keithley 2400 source meter unit under AM1.5G (100 mW cm^{-2}) spectrum from a solar simulator. The incident photon to current conversion efficiency (IPCE) spectra of the PSCs were recorded using Bentham IPCE system (model 300).

The hole mobility and electron mobility of the blended films were estimated by recording the under dark J-V characteristics of *hole only* (ITO/PEDOT:PSS/active layer/Al) and *electron only* (ITO/Al/active layer/Al) and fitting the data with the space charge limited current (SCLC) model.

Cyclic voltammetry (CV) was performed with a three-electrode-compartment cell in CH_2Cl_2 solutions with 0.1 M $[\text{n-Bu}_4\text{N}](\text{ClO}_4)$ as supporting electrolyte using CHI-730D electrochemistry workstation. A glassy carbon electrode of diameter 3 mm was used as the working electrode while platinum wire and Ag/AgCl electrodes were used as the counter and reference electrodes respectively.

X-ray diffraction (XRD) measurement was carried out using XRD Panalytical make. The thin film of the active layer (SVA treated) were deposited on the glass substrates (100 nm) and measurement was carried out in plane geometry. $\text{CuK}\alpha$ X-radiation is used as incident radiation. Transmission electron microscopy images were recorded on Tecnai G2 20 S-TWIN [FEI 200 Kv TEM equipment].

Table S1. Photovoltaic parameters of the as cast **P:PC₇₁BM** based OSCs with different weight ratios between **P** and **PC₇₁BM**.

P:PC ₇₁ BM weight ratio	J _{SC} (mA/cm ²)	V _{OC} (V)	FF	PCE (%)
1:0.5	12.41	0.77	0.51	4.87
1:1.0	13.76	0.78	0.53	5.69
1:1.4	14.38	0.78	0.56	6.28
1:1.5	13.82	0.79	0.53	5.79

Table S2. Photovoltaic parameters of the as cast **P:Cz-IC** based OSCs with different weight ratios between **P** and **Cz-IC**.

P:Cz-IC weight ratio	J _{SC} (mA/cm ²)	V _{OC} (V)	FF	PCE (%)
1:0.4	13.96	1.01	0.47	6.62
1:0.8	15.17	1.00	0.50	7.58
1:1.2	16.38	1.02	0.52	8.69

1:1.3	15.72	1.01	0.49	7.78
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Table S3. Photovoltaic parameters of the as cast P:PC₇₁BM/Cz-IC ternary OSCs with different weight ratios between PC₇₁BM and Cz-IC.

PC ₇₁ BM:Cz-IC weight ratio	J _{SC} (mA/cm ²)	V _{OC} (V)	FF	PCE (%)
0.1:1.1	18.38	0.96	0.61	10.76
0.2:1.0	19.45	0.95	0.65	12.01
0.3: 0.9	18.38	0.96	0.62	10.94

Table S4. HOMO and LUMO energy levels of the blend with different weight ratios of PC₇₁BM and Cz-IC.

PC ₇₁ BM:Cz-IC (weight ratio)	HOMO (eV)	LUMO (eV)
0:1	-5.98	-3.77
0.2:0.8	-6.02	-3.88
0.4:0.6	-6.06	-3.92
0.6:0.4	-6.08	-4.02
1:0	-6.10	4.12

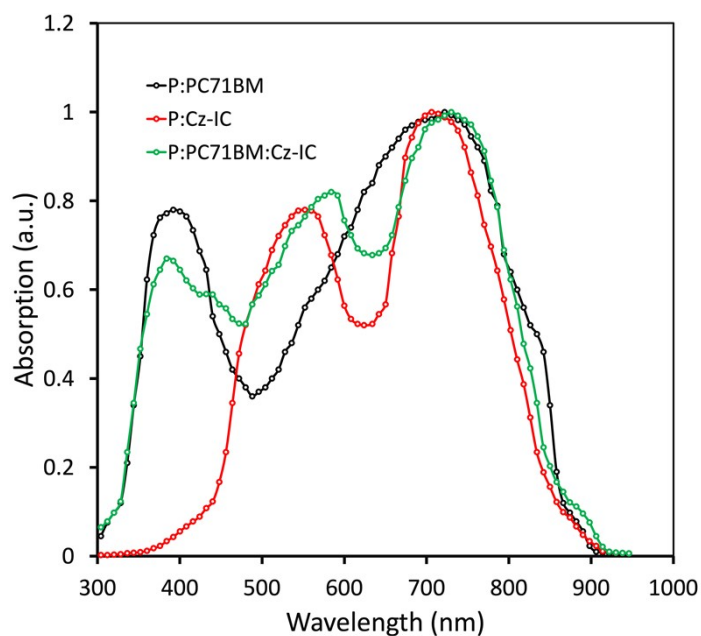


Fig S1. Optical absorption spectra of binary and ternary thin films

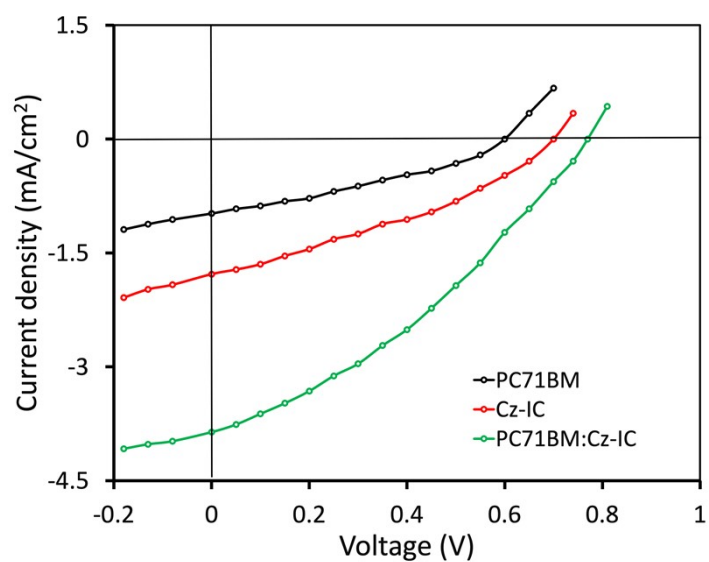


Fig S2. J-V characteristics of the devices based in pristine PC₇₁BM, Cz-IC and PC₇₁:BM:Cz-IC blend as active layer

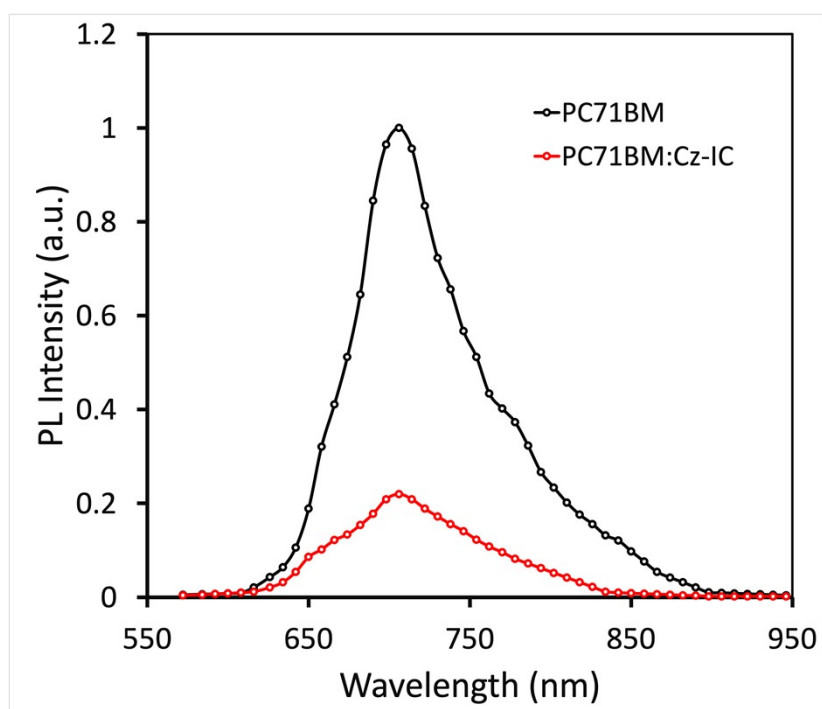


Fig S3. PL spectra of the pristine PC₇₁BM and PC₇₁BM:Cz-IC blend excited at 500 nm.

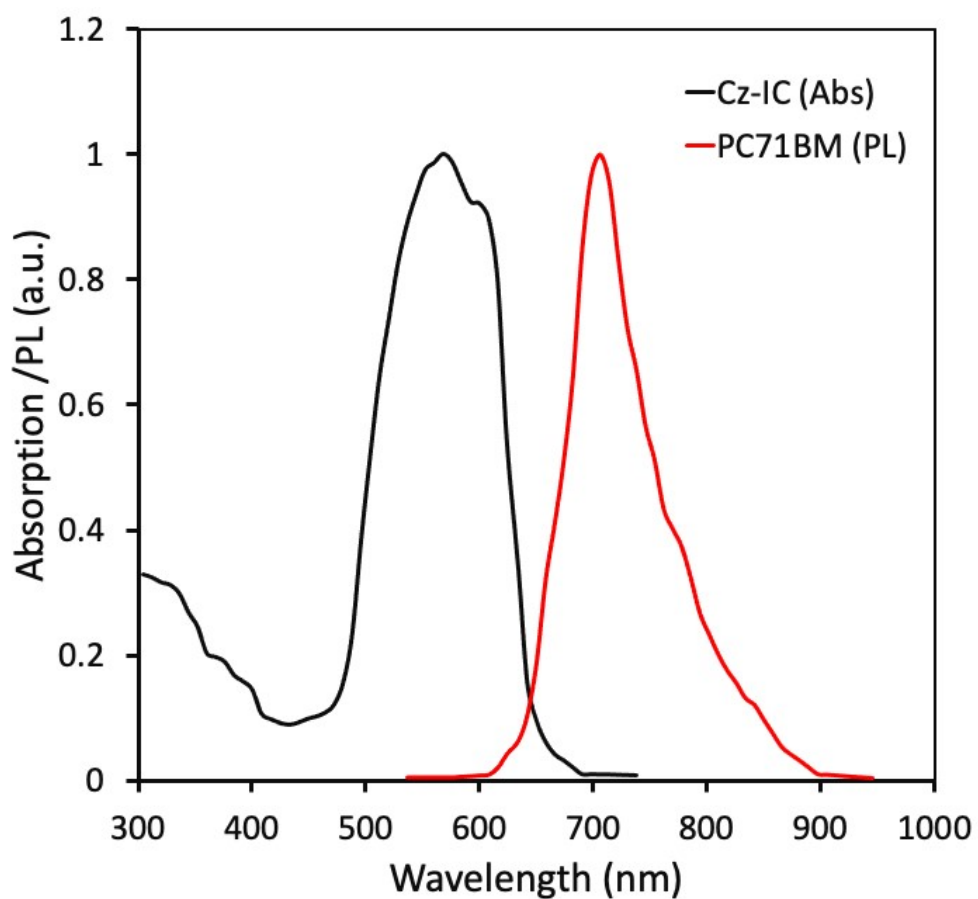


Fig. S4 Absorption spectra (film) of Cz-IC and PL spectra (film) of PC₇₁BM.

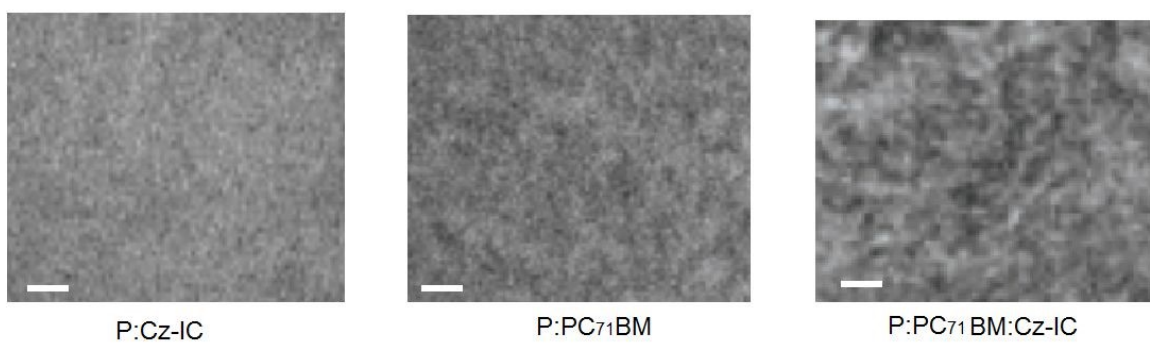


Fig. S5. TEM images of **P:Cz-IC**, **P:PC₇₁BM** and **P:PC₇₁BM/Cz-IC** thin films. Scale bar is 100 nm.