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Improving the Performance of Near Infrared Binary Polymer Solar Cells by Adding Second Non-fullerene Intermediate Band-gap Acceptor

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Characterization

UV-vis absorption spectra were measured using a Shimadzu UV-2500 recording spectrophotometer. Cyclic voltammetry (CV) measurements of targeted SMA thin films were conducted on a CHI voltammetric analyzer in acetonitrile solution with 0.1 M tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6) as supporting electrolyte at room temperature by using a scan rate of 100 mV s^{-1} and conventional three-electrode configuration.

AFM measurements were obtained by using a Dimension Icon AFM (Bruker) in a tapping mode. The grazing incidence X-ray scattering (GIWAXS) measurement was carried out with a Xeuss 2.0 SAXS/WAXS laboratory beamline using a Cu X-ray source (8.05 keV, 1.54 Å) and a Pilatus3R 300K detector. The incident angle was 0.2°. The samples for GIWAXS/GISAXS measurements were fabricated on silicon substrates using the same recipe for the devices.

Solar cell fabrication and characterization

Solar cells were fabricated in a conventional device configuration of ITO/PEDOT:PSS/active layers/PNDIT-F3N/Ag. The ITO substrates were first scrubbed by detergent and then sonicated with deionized water, acetone and isopropanol subsequently, and dried overnight in an oven. The glass substrates were treated by UV-Ozone for 30 min before use. PEDOT:PSS (Heraeus Clevios P VP AI 4083) was spin-cast onto the ITO substrates at 4000 rpm for 30 s, and then dried at 150 °C for 15 min in air. The PBDB-T-2Cl: acceptor blends (1:1 weight ratio) were dissolved in chloroform (the total concentration of blend solutions was 16 mg mL^{-1} for all blends), and stirred overnight on a hotplate at 40°C in a nitrogen-filled glove box. The blend solution was spin-cast at 2700 rpm for 30 s. A thin PNDIT-F3N layer was coated on the active layer, followed by the deposition of Ag (100 nm) (evaporated under 5×10^{-5} Pa through a shadow mask). The optimal active layer thickness measured by a Bruker Dektak XT stylus profilometer was about 100 nm. The current density-voltage (J-V) curves of all encapsulated devices were measured using a Keithley 2400 Source Meter in air under AM 1.5G (100 mW cm-2) using a Newport solar simulator. The light intensity was calibrated using a standard Si diode (with KG5 filter, purchased from PV Measurement to bring spectral mismatch to unity). Optical microscope (Olympus BX51) was used to define the device area (4.6 mm²). EQEs were measured using an Enlitech QE-S EQE system equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

SCLC measurements

The electron and hole mobility were measured by using the method of space-charge limited current (SCLC) for electron-only devices with the structure of ITO/ZnO/active layer/PNDIT-F3N/Ag and hole-only devices with the structure of ITO/MoO_x/active layers/MoO_x/Ag. The charge carrier mobility was determined by fitting the dark current to the model of a single carrier SCLC according to the equation: $J = 9\varepsilon_0\varepsilon_r\mu V^2/8d^3$, where J is the current density, d is the film thickness of the active layer, μ is the charge carrier mobility, ε_r is the relative dielectric constant of the transport medium, and ε_0 is the permittivity of free space. $V = V_{app} - V_{bi}$, where V_{app} is the applied voltage, V_{bi} is the offset voltage. The carrier mobility can be calculated from the slope of the $J^{1/2} \sim V$ curves.

Atomic force microscopy (AFM). AFM images were obtained by using a Dimension Icon AFM (Bruker) in a tapping mode.

GIWAXS characterization. GIWAXS measurement were carried out with a Xeuss 2.0 SAXS/WAXS laboratory beamline using a Cu X-ray source (8.05 keV, 1.54 Å) and a Pilatus3R 300K detector. The incidence angle is 0.2°. The samples for GIWAXS measurements are fabricated on silicon substrates using the same recipe for the devices.

GISAXS characterization. GISAXS was conducted at 19U2 SAXS beamline at Shanghai Synchrotron Radiation Facility, Shanghai, China, using the 0.15° incident angle with 10 keV primary beam.

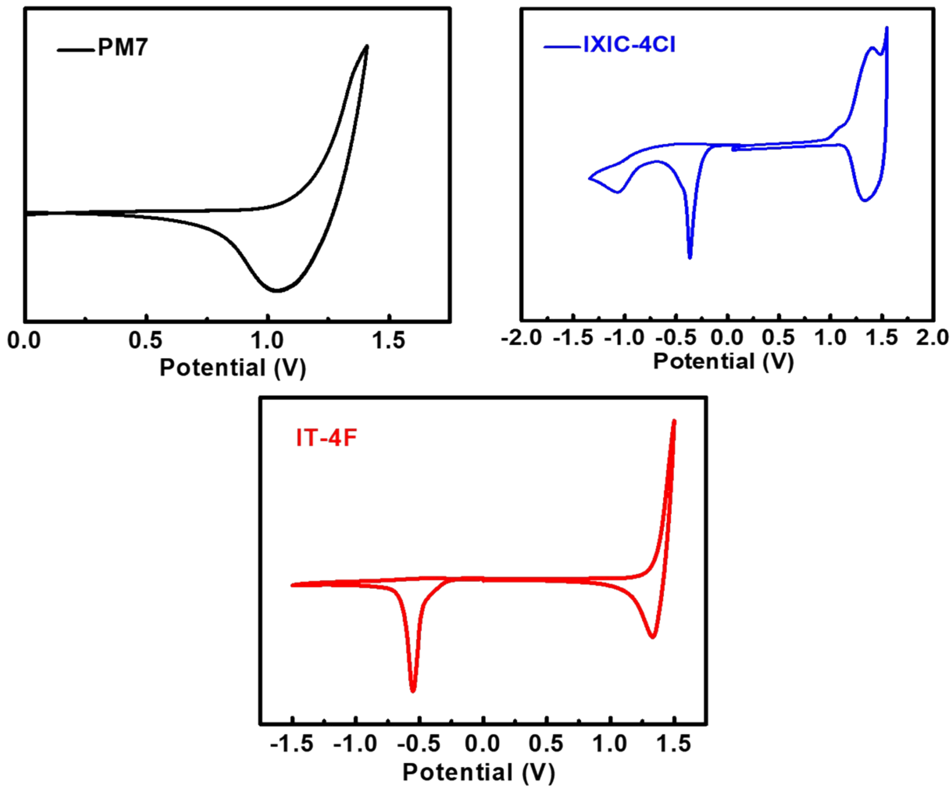

Figure S1. The CV curves of PBDB-T-2Cl, IXIC-4Cl and IT-4F

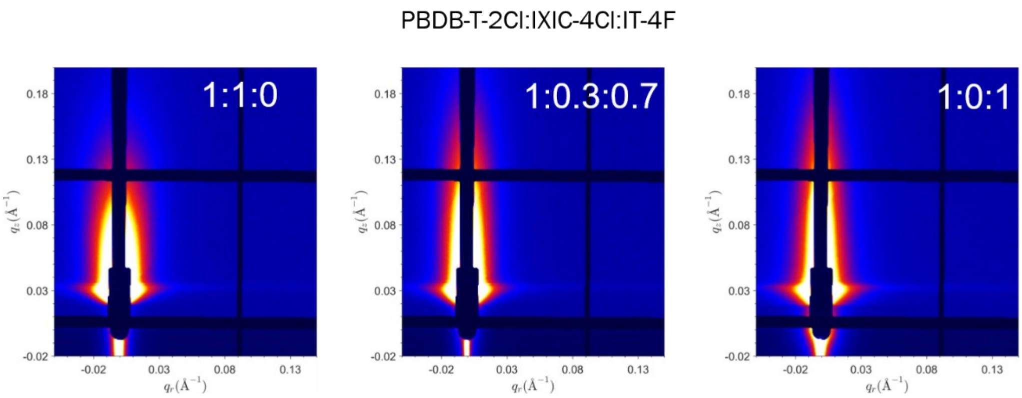

Figure S2. 2D GISAXS patterns of the ternary blend films with different weight ratios of PBDB-T-2Cl:IXIC-4Cl:IT-4F system.

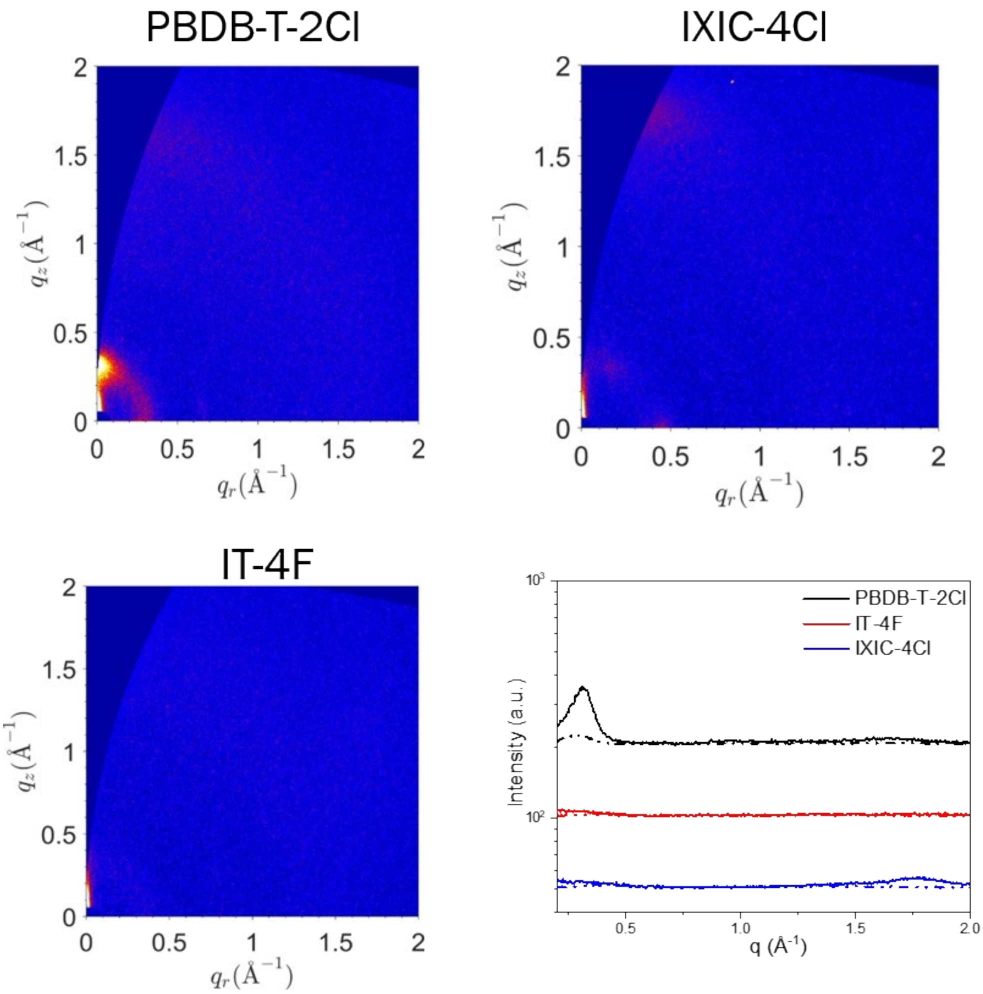

Figure S3. GIWAXS patterns of PBDB-T-2Cl, IXIC-4Cl and IT-4F neat film, and the out-of-plane (dotted lines) and in-plane (solid lines) line-cut profiles of GIWAXS patterns.

Table S1. The parameters of exciton dissociation efficiency and charge collection efficiency.

PBDB-T-2Cl:IXIC-4Cl:IT-4F	J_{sat} (mA cm^{-2})	J_{ph}^{a} (mA cm^{-2})	J_{ph}^{b} (mA cm^{-2})	η_{diss} (%)	η_{coll} (%)
1:1:0	23.906	21.907	18.731	91.6	78.4
1:0.5:0.5	25.299	23.665	20.804	93.5	82.2
1:0.3:0.7	25.064	23.655	21.073	94.4	84.1
1:0:1	20.591	19.941	17.648	96.8	85.7

a: Under short circuit condition; b: Under the maximal power output condition

Table S2. The hole and electron mobility of PBDB-T-2Cl:IXIC-4Cl:IT-4F blend films with different IT-4F contents.

IT-4F contents	μ_h ($cm^2\ V^{-1}\ s^{-1}$)	μ_e ($cm^2\ V^{-1}\ s^{-1}$)	μ_h/μ_e
0%	8.41×10^{-4}	4.35×10^{-4}	1.93
70%	7.10×10^{-4}	4.22×10^{-4}	1.68
100%	6.34×10^{-4}	4.10×10^{-4}	1.55