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Supporting Information

Ternary non-fullerene polymer solar cells with efficiency of 11.6% by simultaneously optimizing photon harvesting and phase separation

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Device fabrication and characterization

The patterned indium tin oxide (ITO) coated glass substrates (15 Ω per square) were successively cleaned by ultrasonic treatment in detergent, de-ionized and ethanol, respectively. The cleaned ITO substrates were further dried by high purity nitrogen and treated by oxygen plasma for 1 min to improve their work function and clearance. Subsequently, poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS, purchased from H.C. Starck co. Ltd.) solution was spin-coated on ITO substrates at 5000 RPM for 40 s and baked at 150 °C for 15 min in atmospheric air. Then ITO substrates coated with PEDOT:PSS films were transferred into a high-purity nitrogen-filled glove box to fabricate active layers. The used materials J71, ITIC (purchased from Solarmer Materials Inc) and MeIC2 (synthesized by Yang's group) were dissolved in chloroform to prepare 18 mg/ml blend solutions. The proportions of ITIC:MeIC2 are 1:0, 0.9:0.1, 0.8:0.2, 0.7:0.3, 0.5:0.5, 0:1 and the weight ratio of acceptor to donor is kept constant as 1:1. After continuouslystirred for 4 hours, The mixed solutions were spin-coated onto the PEDOT:PSS modified ITO substrates at 2000 RPM for 40 s to prepare the active layers. Then The prepared active layers were suffered from different post-treatments: i) chloroform solvent vapor annealing at 1 min. ii) thermal annealing at 150 ℃ for 5 min; the prepared PDIN solutions were spin-coated onto the active layers at 5000 RPM for 35s. Finally, 100nm aluminum (Al) were deposited by thermal evaporation with a shadow mask in the vacuum condition of 10^{-5} Pa. The active area is approximately 3.8 mm^2, which is defined by the overlapping area of ITO anode and Al cathode.

The current density-voltage (*J*-*V*) curves of all PSCs were measured by a Keithley 2400 unit in high-purity nitrogen-filled glove box. The AM 1.5G irradiation was provided by an XES-40S2 (SAN-EI ELECTRIC Co., Ltd) solar simulator (AAA grade, 70×70 mm^2 photobeam size) with light intensity of 100 mW/cm^2. The external quantum efficiency (EQE) spectra of organic solar cells were measured by a Zolix Solar Cell Scan 100. The absorption spectra of films were measured with a Shimadzu UV-3101 PC spectrometer. The photoluminescence (PL) spectra of films and solutions were measured by a HORIBA Fluorolog®-3 spectrofluorometer system. Transmission

electron microscopy (TEM) images of active layers were obtained by a JEOL JEM-1400 transmission electron microscope operated at 80 kV. The HOMO/LUMO levels of J71 and ITIC are cited from the references, which were measured by Cyclic Voltammetry (CV) method. The HOMO/LUMO levels of MeIC2 were measured by Cyclic Voltammetry (CV), these measurements were carried out on a CHI Voltammetric Analyzer at room temperature. Tetrabuty-lammonium hexafluorophosphate (n-Bu4NPF6, 0.1 M) was used as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode with a 2 mm diameter, a platinum wire counter electrode, and a Ag/AgCl wire reference electrode. The C-V curves were obtained at a scan rate of 100 mV s-1. The potentials were determined using ferrocene as the reference. The HOMO and LUMO energy levels were calculated according to the following equations:

$$HOMO = -[E_{ox} + (4.80 - E_{Fc})]\text{eV};$$
$$LUMO = -[E_{red} + (4.80 - E_{Fc})]\text{eV};$$

where E_{ox} and E_{red} are the onset of oxidation and reduction potential, respectively.

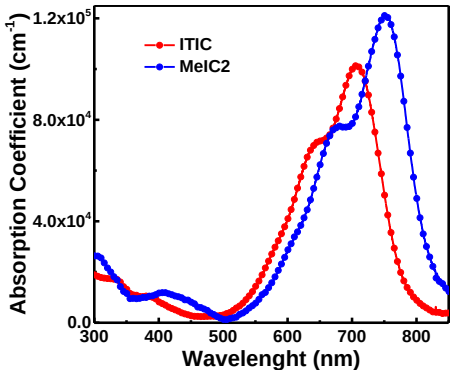

Figure S1. Absorption coefficients spectra of neat MeIC2 and ITIC films.

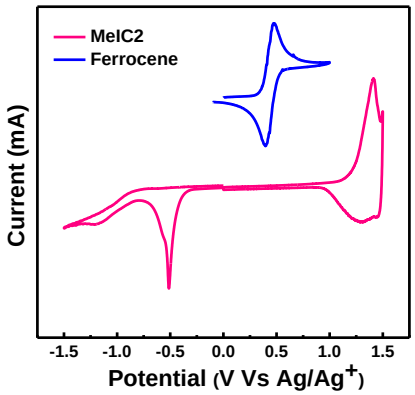

Figure S2. *C-V* plot of MeIC2 film. The E_{Fe} E_{ox} and E_{red} extracted from the *C-V* curve are 0.435 V, 1.1954 V, -0.4050 V.

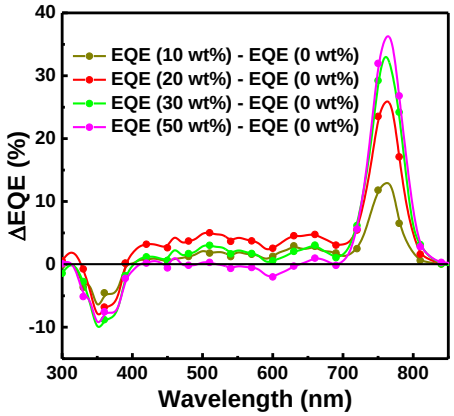

Figure S3. ΔEQE spectra between ternary PSCs and ITIC based binary PSCs.

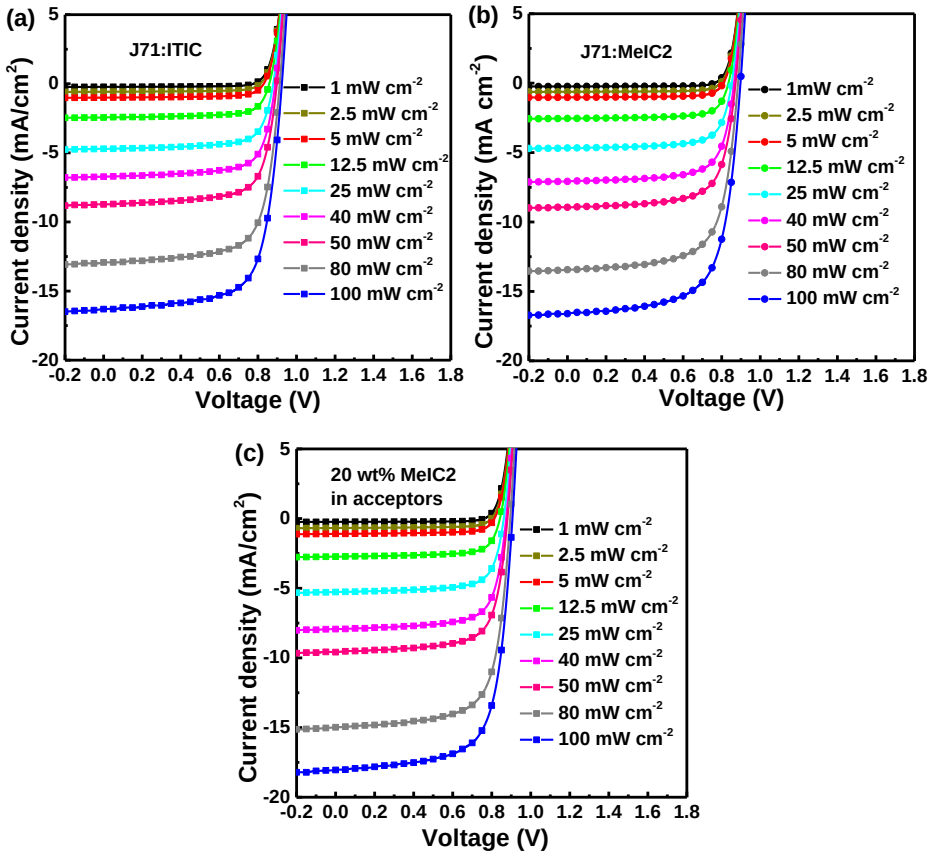

Figure S4. The *J-V* curves (a) and (b) of J71 based binary and (c) the optimized ternary PSCs under different light illumination intensity.

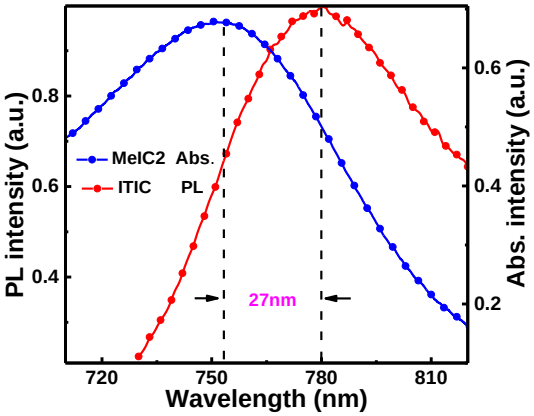

Figure S5. Normalized PL spectrum of neat ITIC film and absorption spectrum of neat MeIC2 film.

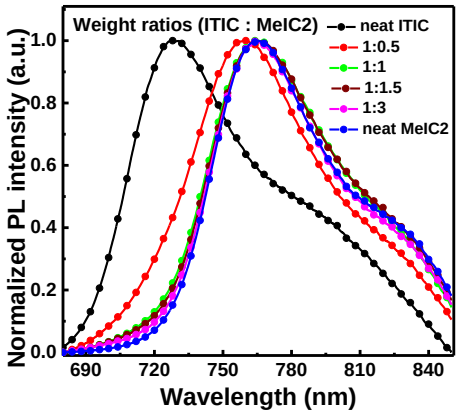

Figure S6. Normalized PL spectra of neat ITIC, MeIC2 and blend ITIC:MeIC2 solutions with different weight ratios under 660 nm light excitation.