Efficient inverted perovskite solar cells with truxene-bridged PDI trimers as electron transporting materials

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Experimental section

Materials and instruments

Unless otherwise stated, all starting materials were purchased from commercial suppliers (Sigma-Aldrich and Energy Chemical) and used without further purification, including P3CT (Rieke Metals), PbI_2 (p-OLED, >99.99 %), MAI (p-OLED, ≥99.5 %), PCBM (p-OLED, ≥99 %), C_{60} (p-OLED), BCP (p-OLED), DMF (Sigma-Aldrich, 99.8 %), DMSO (Sigma-Aldrich, 99.8 %) and CB (Sigma-Aldrich, 99.8 %). UV/Vis absorption spectra were recorded on a Shimadzu UV-2450 absorption spectrophotometer. Fluorescence spectra were measured on a Hitachi F-4600 FL Spectrophotometer. The PL lifetimes were measured by a single photon counting spectrometer from Edinburgh Instruments (FLS920) with a Picosecond Pulsed UV-LASTER (LASTER377) as the excitation source. Field-emission SEM (FE-SEM) image was taken on JSM-7800F. Cyclic voltammetry (CV) was carried out in 0.1 M dichloromethane solution using $TBAPF_6$ as the electrolyte. The curves were recorded using the SCE as the reference electrode, and they were calibrated by the ferrocene-ferrocenium (Fc/Fc^+) redox couple, with a scanning rate of 100 mV s^{-1}. AFM images were collected in air on a Bruker AFM using a tapping mode.

Device fabrication

The devices were fabricated according to our previous work. The indium tin oxide (ITO) glass substrates were sequentially washed by sonication using detergent, deionized water, ethanol and acetone. The hole transporting layer P3CT-Na was formed on ITO substrates by spin coating at 4000 rpm for 60 s followed by annealing at 140°C for 30 min. Then the samples were transferred into a N_2-filled glovebox. A $CH_3NH_3PbI_3$ precursor solution (1.4 M in DMF: DMSO mixed solution with a v/v of 4:1) was spin-coated in a two-step program at 400 and 5000 rpm for 3 and 30 s, respectively. During the second step, 200 μL of chlorobenzene was poured on the spinning substrate at 10 s after the start-up. Next, the as-spun perovskite layer was annealed on a hot plate at 60 °C for 1 min and at 80 °C for 2 min to drive off solvent and form the perovskite phase. Then Tr-PDI derivative in chlorobenzene were spin-coated (5000 rpm) onto the perovskite layer. To fabricate ITO/P3CT-Na/Perovskite/ETL/BCP/Ag device, 6 nm thick BCP was then thermally evaporated, and an approximately 100 nm thick Ag counter electrode was deposited on top to finish the device fabrication. To fabricate ITO/P3CT-Na/Perovskite/Tr-PDI_3 or Tr-PDI_3-C/C_{60}/BCP/Ag device, C_{60} (40 nm) and BCP (6 nm) were evaporated under high vacuum on top of the interlayer. Finally, a 100 nm thick Ag electrode was deposited through a shadow mask. The active area of our device is 0.09 cm^2.

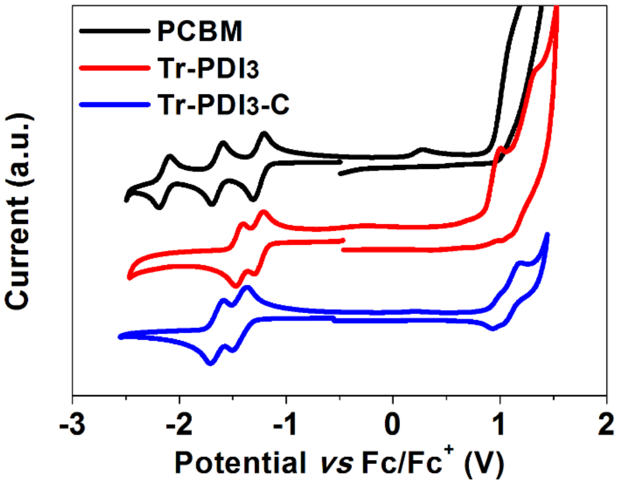

Figure S1. Cyclic voltammograms of PCBM, Tr-PDI$_3$ and Tr-PDI$_3$-C.

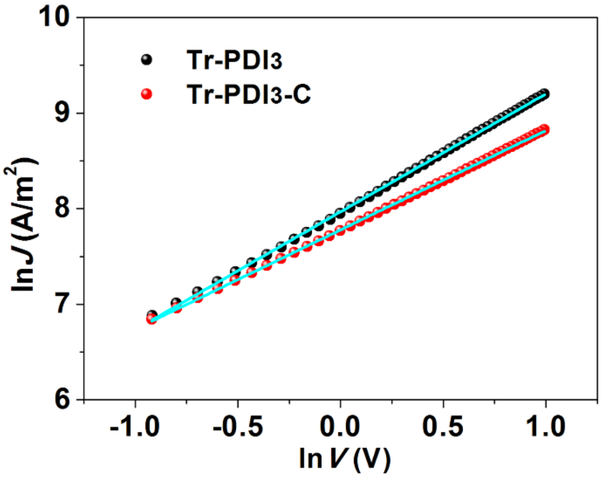

Figure S2. The current-voltage data of SCLC model based on the configuration of ITO/ZnO/Tr-PDI$_3$ or Tr-PDI$_3$-C/BCP/Ag.

Table S1. The photovoltaic parameters of the device with Tr-PDI$_3$ ETL in different thicknesses.

Tr-PDI$_3$	V_{OC} (mV)	J_{SC} (mA cm^{-2})	FF	PCE (%)
48 nm	1041	20.90	0.71	15.51
31 nm	1032	21.47	0.79	17.45
23 nm	1035	21.07	0.77	16.77
17 nm	1033	20.83	0.66	14.27

Table S2. The photovoltaic parameters of the device with Tr-PDI$_3$-C ETL in different thicknesses.

Tr-PDI$_3$-C	V_{OC} (mV)	J_{SC} (mA cm^{-2})	FF	PCE (%)
46 nm	1049	20.03	0.64	13.48
33 nm	1050	20.52	0.75	16.09
25 nm	1047	20.92	0.77	16.90
16 nm	1041	20.35	0.71	15.10

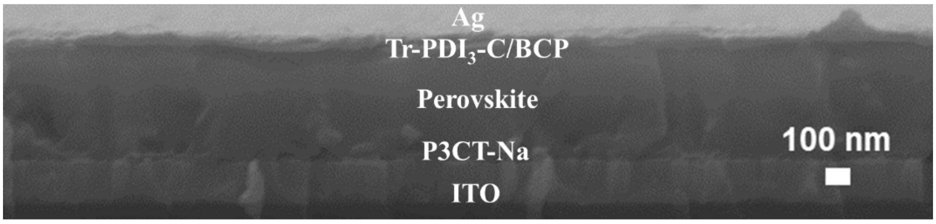

Figure S3. Cross-sectional SEM image of inverted PSCs.

Table S3. Photovoltaic parameters of the inverted devices with Tr-PDI$_3$ or Tr-PDI$_3$-C ETL under forward and reverse scan directions, respectively.

ETLs	Scan direction	V_{OC} (mV)	J_{SC} (mA cm^{-2})	FF	PCE (%)
Tr-PDI$_3$/BCP	forward	1030	21.39	0.78	17.27
	reverse	1032	21.47	0.79	17.45
Tr-PDI$_3$-C/BCP	forward	1045	20.92	0.76	16.66
	reverse	1047	20.92	0.77	16.90

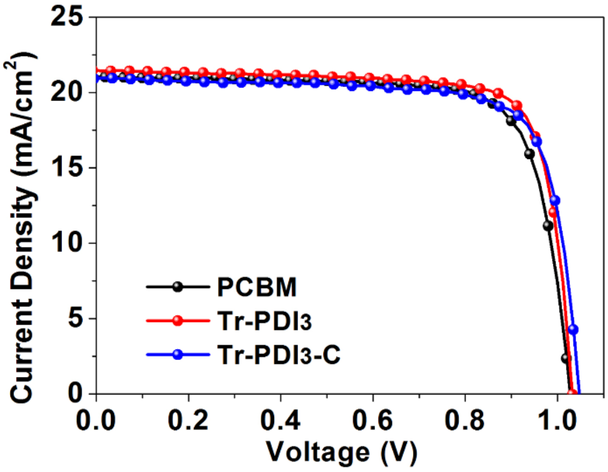

Figure S4. *J-V* curves of PSCs based on PC$_{61}$BM, Tr-PDI$_3$ and Tr-PDI$_3$-C as the ETL, respectively.

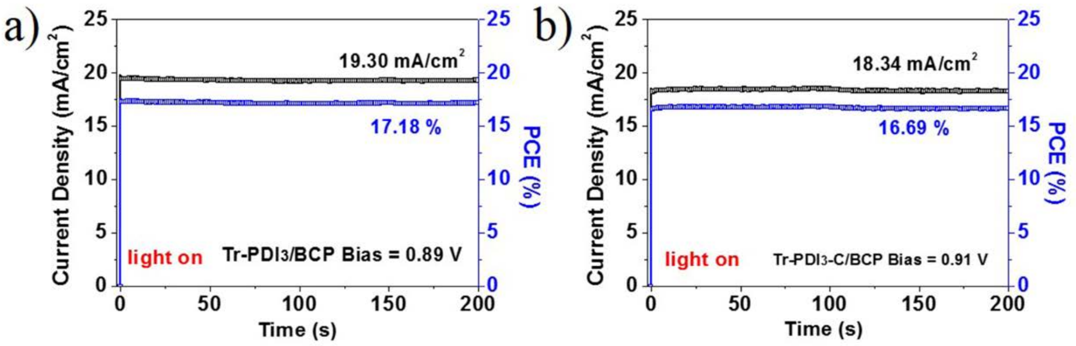

Figure S5. Steady-state J_{SC} and efficiency output of devices using (a) Tr-PDI$_3$ and (b) Tr-PDI$_3$-C as the ETL, respectively.

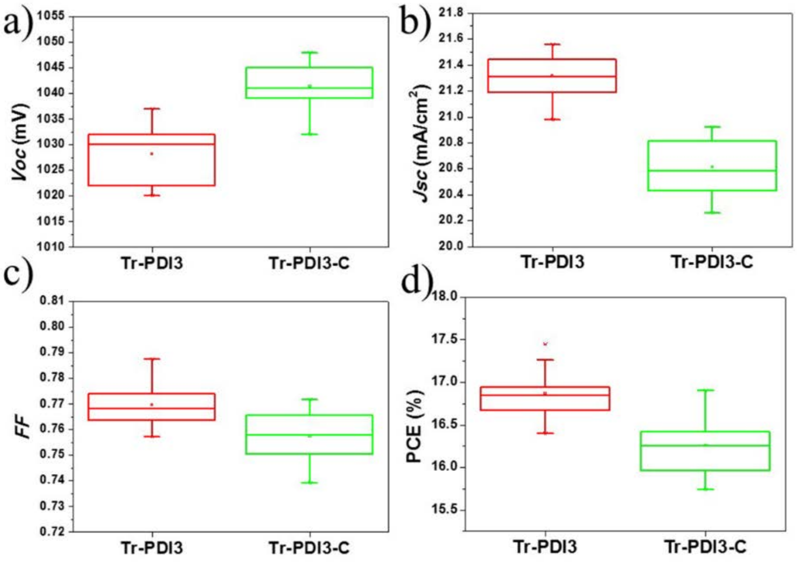

Figure S6. Statistics of photovoltaic parameters (a) V_{OC}, (b) J_{SC}, (c) FF, and (d) PCE of 20 PSCs containing Tr-PDI$_3$ or Tr-PDI$_3$-C ETL measured under AM 1.5 G illumination (100 mW cm^{-2}).

Table S4. Photovoltaic parameters of the inverted devices with Tr-PDI$_3$ and Tr-PDI$_3$-C interlayer under forward and reverse scan directions, respectively.

ETLs	Scan direction	V_{OC} (mV)	J_{SC} (mA cm^{-2})	FF	PCE (%)
Tr-PDI$_3$/C$_{60}$/BCP	forward	1078	22.21	0.82	19.68
	reverse	1081	22.22	0.83	19.83
Tr-PDI$_3$-C/ C$_{60}$/BCP	forward	1083	21.98	0.80	19.14
	reverse	1086	21.97	0.81	19.24

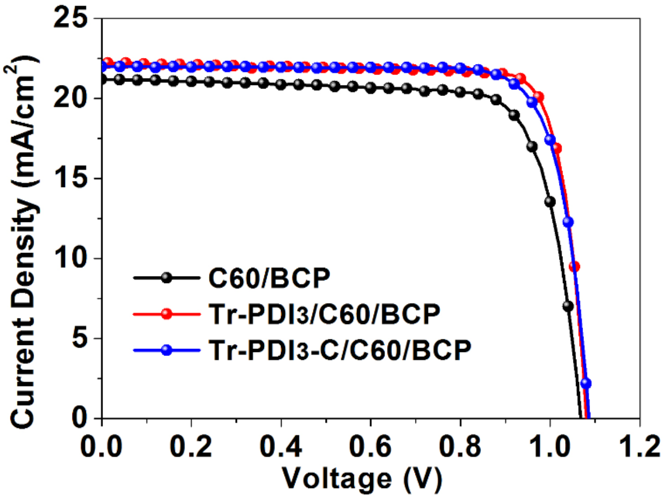

Figure S7. *J-V* curves of PSCs based on Tr-PDI$_3$ or Tr-PDI$_3$-C interlayer and compared with the control device.

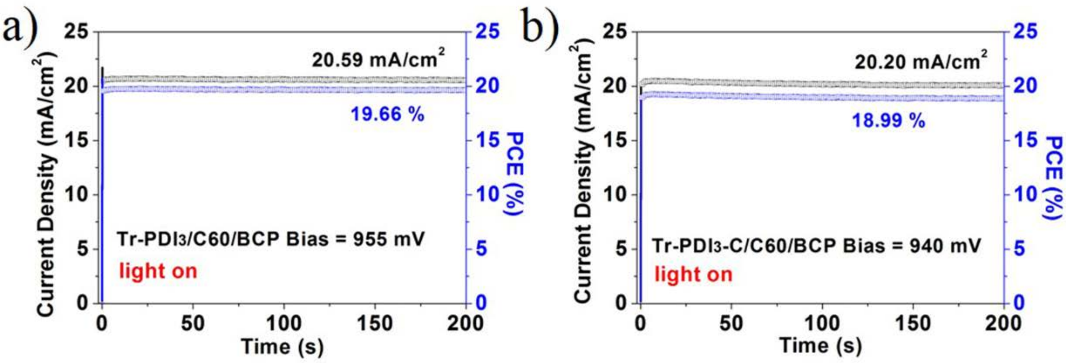

Figure S8. Steady-state J_{SC} and efficiency output of the device with (a) Tr-PDI$_3$ and (b) Tr-PDI$_3$-C interlayer, respectively.

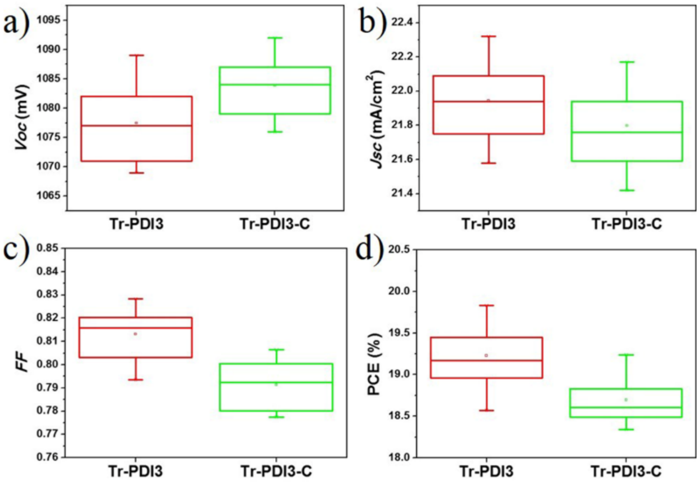

Figure S9. Statistics of photovoltaic parameters (a) V_{OC}, (b) J_{SC}, (c) FF, and (d) PCE of 20 PSCs containing Tr-PDI$_3$ or Tr-PDI$_3$-C interlayer measured under AM 1.5 G illumination (100 mW cm^{-2}).

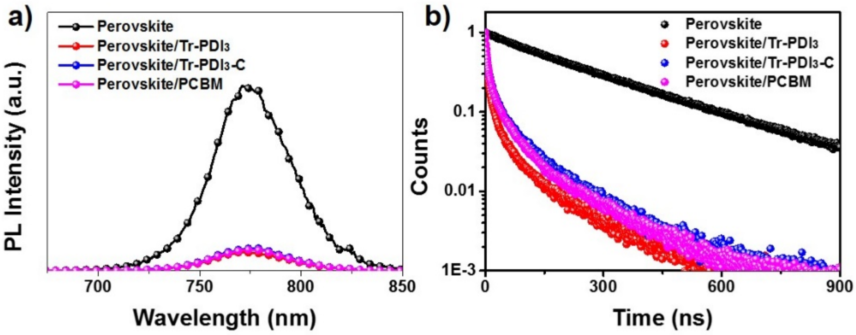

Figure S10. (a) Steady-state and (b) time-resolved PL spectra of neat perovskite, perovskite/PCBM, perovskite/Tr-PDI3 and perovskite/Tr-PDI3-C films, respectively.