



Journal Name

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Supplementary Information

Incorporating deep electron traps in perovskite devices: towards high efficiency solar cells and fast photodetectors

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Experimental details

Materials

The PEDOT:PSS, lead iodine (PbI₂) and methylammonium iodide (CH₃NH₃I) were attained from Xi'an *p*-OLED Co. (China). The m-MTDATA, BCP and C₆₀ were purchased from Lumtec corp. (Taiwan). F4-TCNQ was got from Sigma-Aldrich (UK). All materials were used as received.

Fabrication of devices

The pre-cleaned ITO substrates were firstly treated with UV-ozone for 10 min before use. The m-MTDATA was dissolved into chlorobenzene (CB) with the concentration of 4 mg mL⁻¹, and different contents of F4-TCNQ were added to get the composite solutions with the concentrations of 0.002, 0.005, 0.01, 0.02 and 0.05 mg mL⁻¹ for F4-TCNQ, respectively. The pristine m-MTDATA solution and m:F composite solutions were deposited onto the ITO substrates at 3000 rpm for 50 s, and then annealed at 100 °C for 10 min. The PEDOT:PSS HTL was prepared on the ITO electrode and annealed at 120 °C for 20 min. Subsequently, the perovskite layer was spin-coated onto different HTLs at 4000 rpm and cleaned by anhydrous ether. Finally, the devices were completed by successively evaporating the C₆₀ (30 nm), BCP (9 nm) and Ag (80 nm) onto the perovskite layer. The effective area of device is 0.044 cm².

Film and Device Characterization

The light transmission and absorbance spectra were measured on a Shimadzu UV-1700 spectrophotometer. The surface morphologies were analyzed by a Bruker Dimension Icon AFM. The surface WFs were measured by extracting 100 points in a size of 50×50 μm using a Kelvin probe system. The light *J-V* characteristics were carried out using a Keithley 2601 source meter with an Oriel 300 W solar simulator intensity of ~100 mW cm⁻². The EQE spectra were measured using a Crowntech QTest Station 1000 AD. The surface and cross-sectional morphologies were characterized by a JEOL JSM-7500 field-emission SEM. The contact angles were carried out on a Powereach JC2000D contact angle goniometer. The Nyquist plots were measured by a Precision Impedance Analyzer 6500B Series of Wayne Kerr Electronics. The TPC measurements were carried out using a 550 nm nanosecond laser with repeating frequency of 10 Hz.

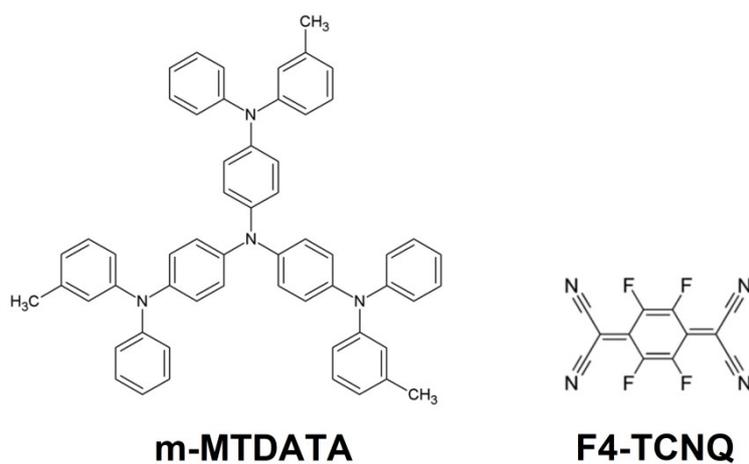


Fig. S1 Chemical structures of m-MTDATA and F4-TCNQ.

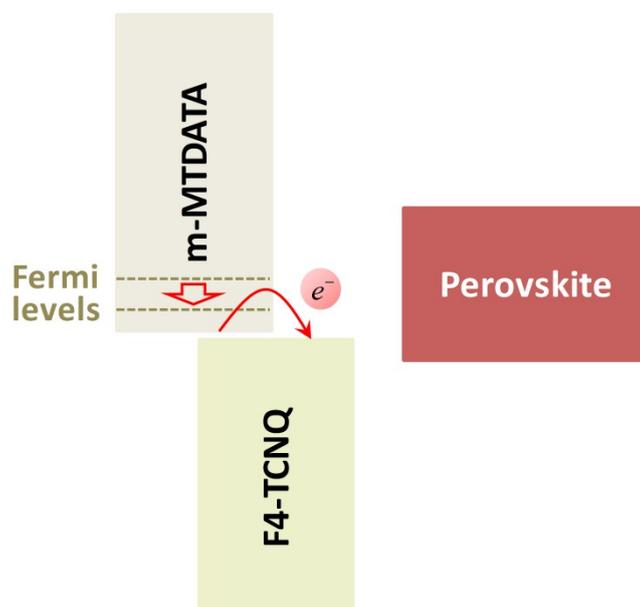


Fig. S2 Electron trapping process in the m:F composite HTL.

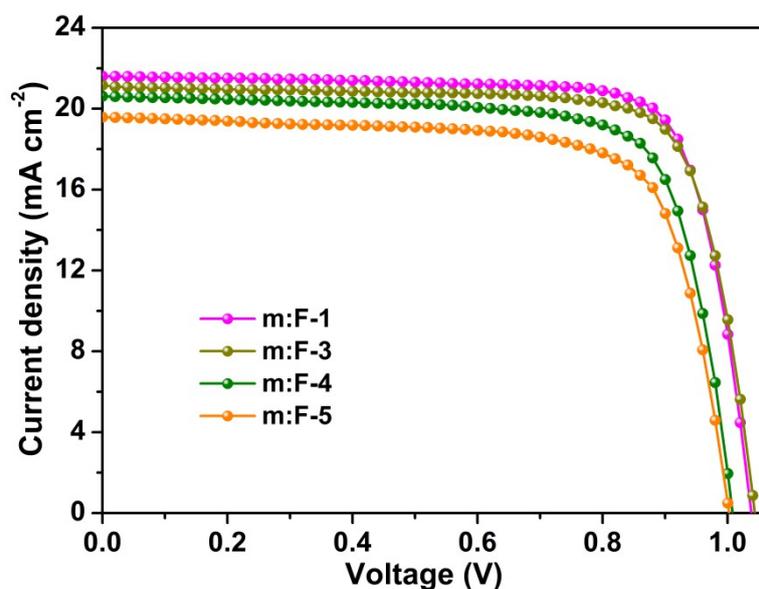


Fig. S3 *J-V* characteristics of devices based on m:F composite HTLs with different doping concentration.

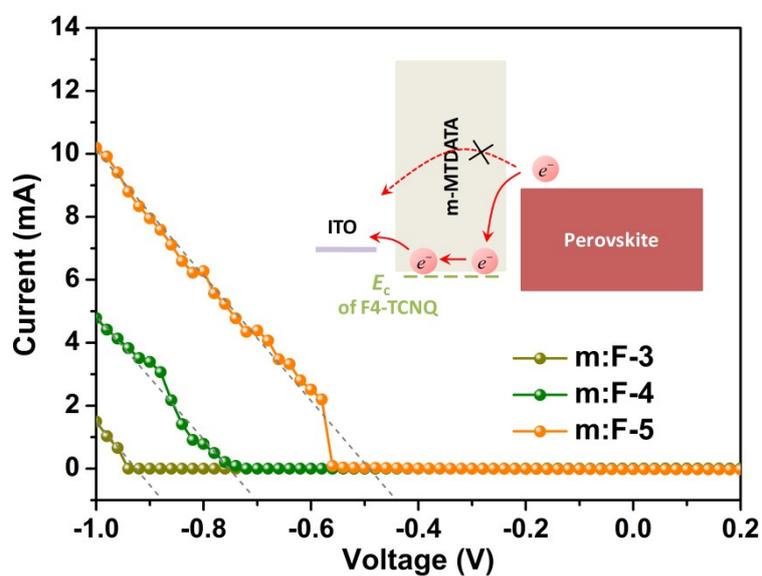


Fig. S4 Dark current-voltage characteristics of devices with m:F-3, m:F-4 and m:F-5, and inset is the charge transport process.

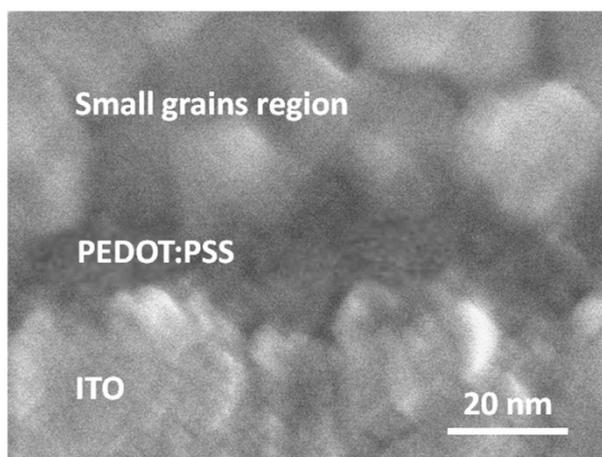


Fig. S5 SEM image of small grains region with higher magnification.

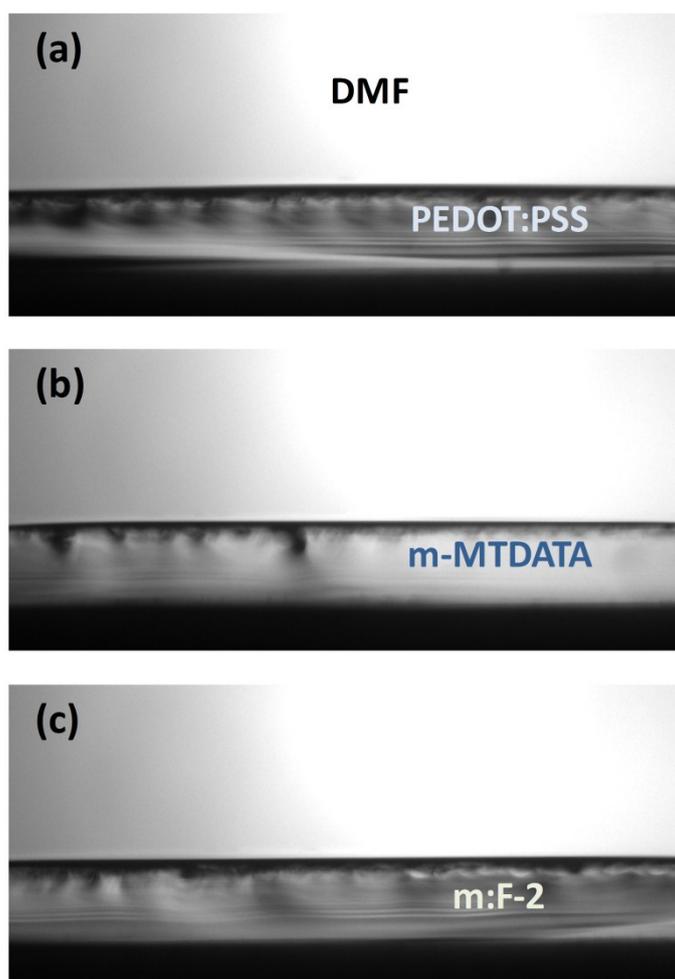


Fig. S6 Contact angles of DMF on PEDOT:PSS, pristine m-MTDATA and m:F-2.

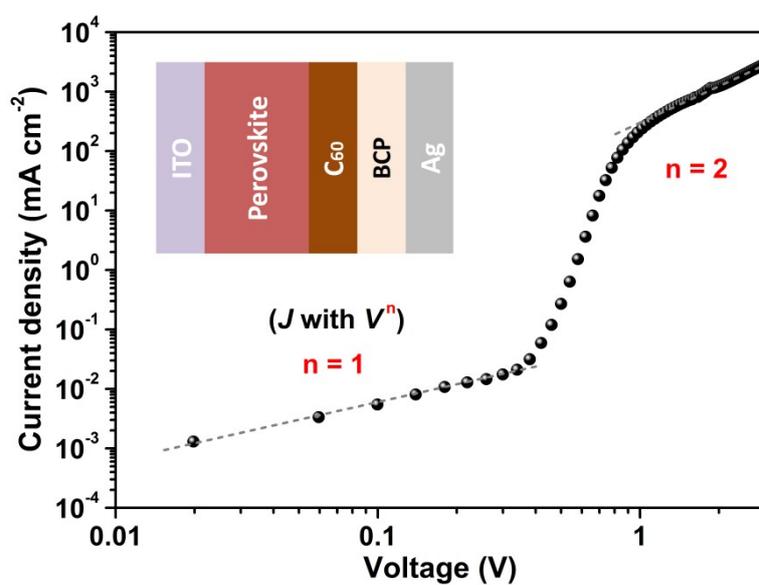


Fig. S7 J - V characteristics of electron-only device, and inset is the device structure.

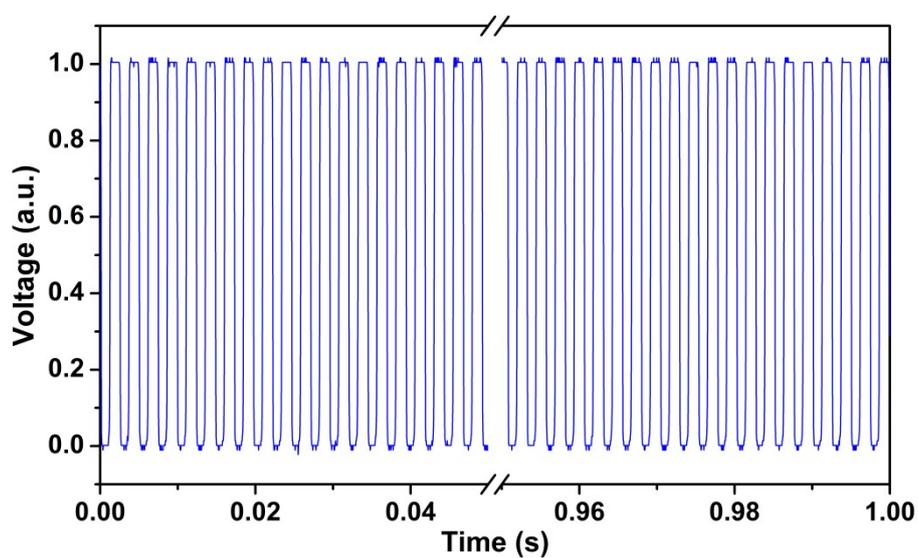


Fig. S8 Multiple time response characteristics of device based on m:F-2 HTL.

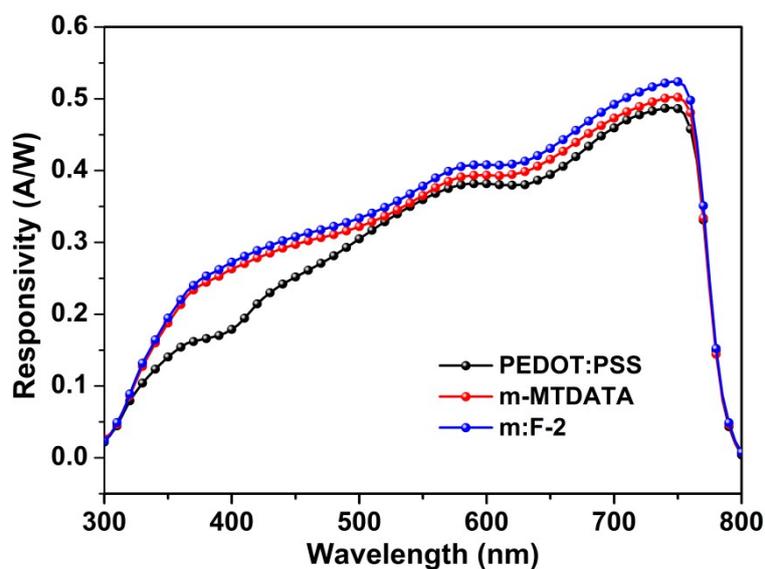


Fig. S9 Spectral R of devices with PEDOT:PSS, pristine m-MTDATA and m:F-2 HTLs.

Table S1 Detail photovoltaic parameters of all devices fabricated here.

HTLs	V_{oc} (V)	J_{sc} (mA cm ⁻²)	Integrated J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)
PEDOT:PSS	0.898	19.33	18.91	78.5	13.63
m-MTDATA	1.026	21.30	20.91	78.4	17.13
M:F-1	1.038	21.61	21.14	78.6	17.63
M:F-2	1.053	22.12	21.69	78.8	18.35
M:F-3	1.043	21.16	20.70	77.7	17.15
M:F-4	1.008	20.61	20.13	75.7	15.73
M:F-5	1.002	19.58	19.09	73.6	14.44