Supplementary Information

Effect of terminal fluorine substitution of nonfullerene small molecular acceptor on the thermal stability of organic solar cells

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1. Materials

Most of chemical reagents and common solvents were purchased from commercial sources. The ITIC, ITIC-4F and polymer PBTIBDTT were synthetized on the basis of the reported papers.

2. Space charge limited current (SCLC) characterization

The carrier mobilities were measured by the space charge limited current (SCLC) method with hole-only devices (ITO/PEDOT:PSS/active layer/Au) and electron only devices (ITO/ZnO/ active layer/PDIN/Al). The measurements of the *I-V* curves were carried out in dark on a computer-controlled Keithley 2400 source-measure unit. The hole and electron mobility was estimated by fitting the *I-V* curves with SCLC model and the Mott-Gurney law: $\ln(I/V^2) = 0.89\beta(V/L)^{1/2} + \ln(9\mu\varepsilon_0\varepsilon S/(8L^3))$. Where I is the current, V is the applied voltage, β is the field activation factor, L is the thickness of films, μ is the mobility, ε_0 is the permittivity of free space, ε is the relative permittivity, and S is the area of films.

3. UV-vis absorption

UV-vis absorption spectra were gained on a Perkin-Elmer UV-vis Lambda 750spectrophotometer (Wellesley, MA).

4. Transmission electron microscopy (TEM)

The TEM images were obtained with a Tecnai G2 F20 high resolution transmission electron microscope operated at an acceleration voltage of 200 KV.

5. Device fabrication

Indium tin oxide (ITO) substrates were cleaned by detergent solution, deionized water, isopropanol and acetone in sequence with ultrasonication, and then treated with UV-ozone for 15 min for further device preparation. Photovoltaic devices were fabricated in traditional structure of ITO/PEDOT:PSS/active layer/PDINO/Al. PEDOT:PSS was spin-coated on the ITO substrates at 3000 rpm for 30s and then baked on a heating equipment at 150 ℃ for 30 min in air. The active layers were spin-coated at 1000-3000 r/min to obtain conceivable films in nitrogen atmosphere, and then treated by spin-coating PDINO from the methanol solution (2 mg mL^{-1}) at 4000 rpm for 30s. Finally, Al was used as cathodes by vapor deposition techniques. The active area of 9 mm^2 and 4 mm^2 was defined by the overlapping of patterned anode and cathode.

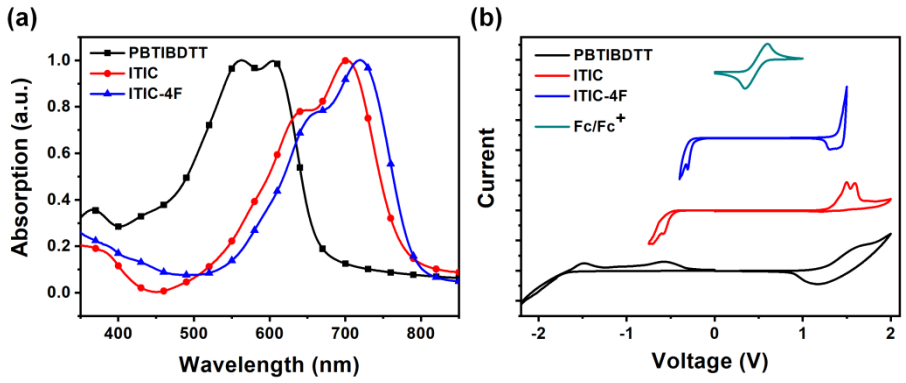

Figure S1. (a) UV−vis absorption spectra of PBTIBDTT, ITIC and ITIC-4F in film. (b) Cyclic voltammogram of PBTIBDTT, ITIC and ITIC-4F.

Table S1. The values of energy levels and optical band gap

molecules	HOMO	LUMO	E_g^{opt}[eV]
PBTIBDTT	-5.47	-3.60	1.86
ITIC	-5.64	-3.86	1.60
ITIC-4F	-5.73	-3.93	1.56

Table S2. The photovoltaic parameters of the devices based on PBTIBDT/ITIC and PBTIBDT/ITIC-4F under illumination of AM 1.5 G, 100 mW cm^{-2}.

Acceptor	D/A ratio	DIO	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF	PCE
ITIC	1:0.8	0%	0.96	13.34	62.10%	7.95%
	1:1	0%	0.98	13.99	65.65%	9.00%
	1:1.2	0%	0.96	13.83	63.40%	8.42%
	1:1	0.25%	0.96	14.14	61.70%	8.37%
ITIC-4F	1:0.7	0%	0.84	16.52	66.06%	9.17%
	1:1	0%	0.86	16.52	65.78%	9.35%
	1:1.4	0%	0.84	16.91	61.11%	8.68%
	1:1	0.5%	0.82	18.17	69.18%	10.31%
	1:1	1%	0.82	17.17	65.64%	9.24%

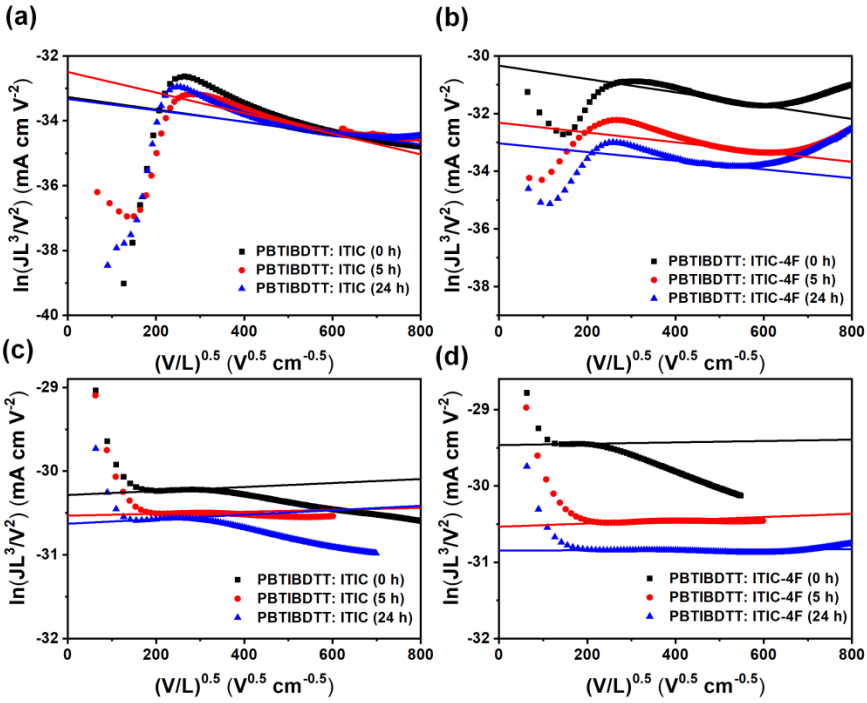

Figure S2. *J–V* characteristics in the dark for (a) hole-only and (c) electron-only devices based on PBTIBDTT/ITIC. J–V characteristics in the dark for (b) hole-only and (d) electron-only devices based on PBTIBDTT/ITIC-4F.

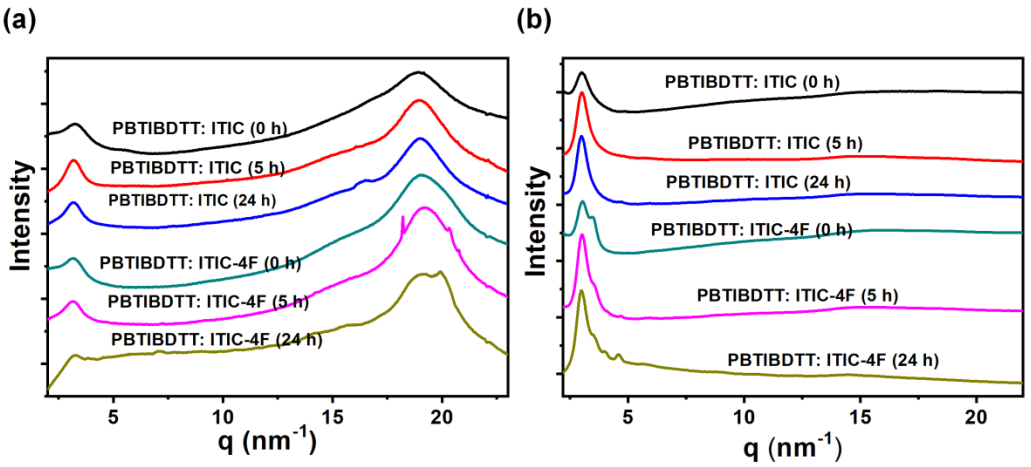

Figure S3. 2D-GIWAXS line-cuts of 2D-GIWAX patterns of blend films based on ITIC and ITIC-4F.