

Supporting information

Alcohol-Soluble Interfacial Fluorenes for Inverted Polymer Solar Cells: Sequence Induced Spatial Conformation Consequently Dipole Moment

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General measurements and characterization.

The nuclear magnetic resonance (NMR) spectra were collected on a Bruker ARX 400 NMR spectrometer with deuterated chloroform as the solvent and with tetramethylsilane ($\delta=0$) as the internal standard. The photoluminescence spectroscopy (PL, Hitachi F-7000), transmittance spectroscopy, UV-vis-NIR spectroscopy, diffuse reflectance spectroscopy (performed by PerkinElmer Lambda 750 with integrating sphere) were utilized. The UPS measurements were carried out in a Thermo-VG Scientific ESCALAB 250 using a He I (21.22 eV) discharge lamp. A bias of -8.0 V was applied to the samples for separation of the sample and the secondary edge for the analyzer. XPS studies were performed on a Thermo-VG Scientific ESCALAB 250 photoelectron spectrometer using a monochromated AlK α (1,486.6 eV) X-ray source. All recorded peaks were corrected for electrostatic effects by setting the C-C component of the C 1s peak to 284.8eV. The base pressure in the XPS analysis chamber was 2×10^{-9} mbar. Atomic force microscopic (AFM) images were measured on a nanoscope III A (Digital Instruments) scanning probe microscope using the tapping mode. TEM images were recorded using a JEOL-2100F transmission electron microscope and an internal charge-coupled device (CCD) camera.

Cyclic voltammetry.

Cyclic voltammetry was performed in an electrolyte solution of 0.1 M tetrabutylammonium hexafluorophosphate in acetonitrile, both working and counter electrodes were platinum electrode. Ag/AgCl electrode was used as thereference electrode (**Figure S1**).

Space-charge-limited-current (SCLC) mobility measurement.

In order to characterize the carrier mobility of modified device, electron-only devices and hole-only devices were fabricated. The electron-only devices used a diode configuration of ITO/ETLs/P3HT:PCBM/LiF/Al The carrier mobility was measured using the SCLC model at low voltage which is described by below Equation:¹

$$J=9\epsilon_0\epsilon_r\mu V^2/8L^3$$

Where ϵ_0 is the permittivity of free space ($8.85 \times 10^{-12} \text{ F}\cdot\text{m}^{-1}$), ϵ_r is the dielectric constant of P3HT or PCBM (assumed to 3), μ is the mobility of an electron, V is the applied voltage, and L is the film thickness.² The thickness of the BHJ blend for SCLC measurement was about 120 nm. By fitting the results to a space-charge-limited form, $J^{0.5}$ versus V is plotted in **Figure 5c**.

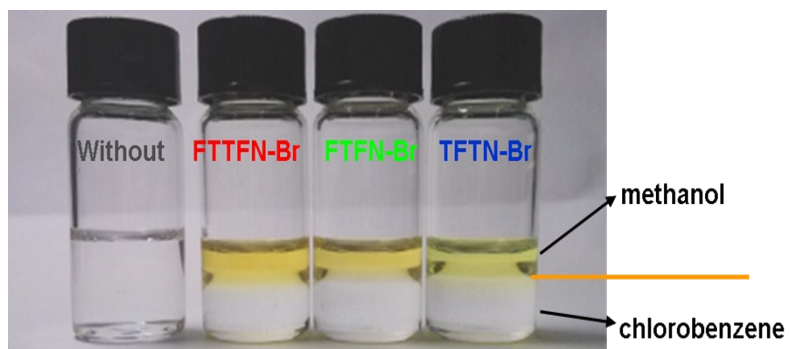


Figure S1. The SMEs dissolved in the methanol/chlorobenzene mixed solution

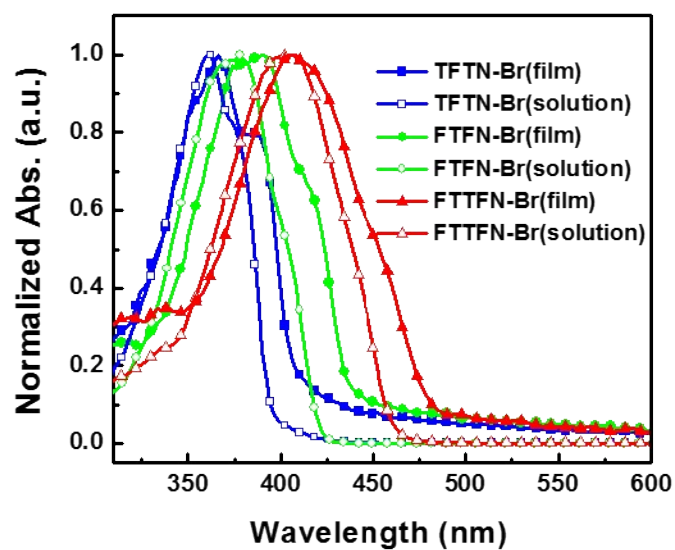


Figure S2. Normalized UV-vis absorption spectra of TFTN-Br, FTFN-Br and FTTFN-Br in their film state and solution

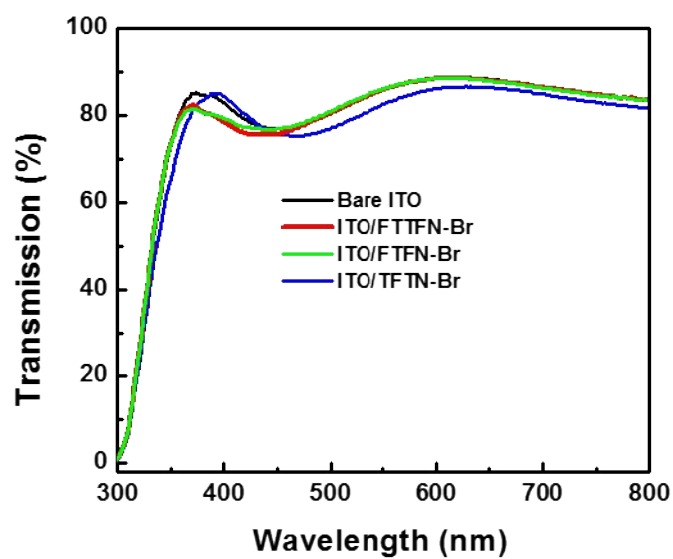


Figure S3. The optical transmittance spectra of the TFTN-Br, FTFN-Br, FTTFN-Br and bare ITO.

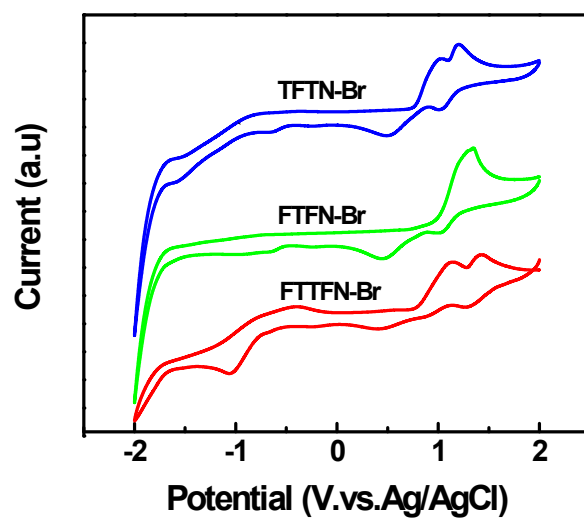


Figure S4. Cyclic voltammogram of TFTN-Br, FTFN-Br and FTTFN-Br films in an acetonitrile solution of 0.1 M Bu_4NPF_6 at a scan rate of 50 mV S^{-1} .

Table S1. Optical and electrochemical properties of the SMEs

compound	$\lambda_{\text{abs, max}}$ (solution) (nm)	$\lambda_{\text{abs, max}}$ (film) (nm)	$E_{\text{g}}^{\text{opt}}$ (eV)	E_{g}^{CV} (eV)	HOMO (eV)	LUMO (eV)
TFTN-Br	361	366	2.95	2.56	-5.16	-2.60
FTFN-Br	378	390	2.81	2.51	-5.34	-2.83
FTTFN-Br	403	411	2.55	2.20	-5.20	-3.00

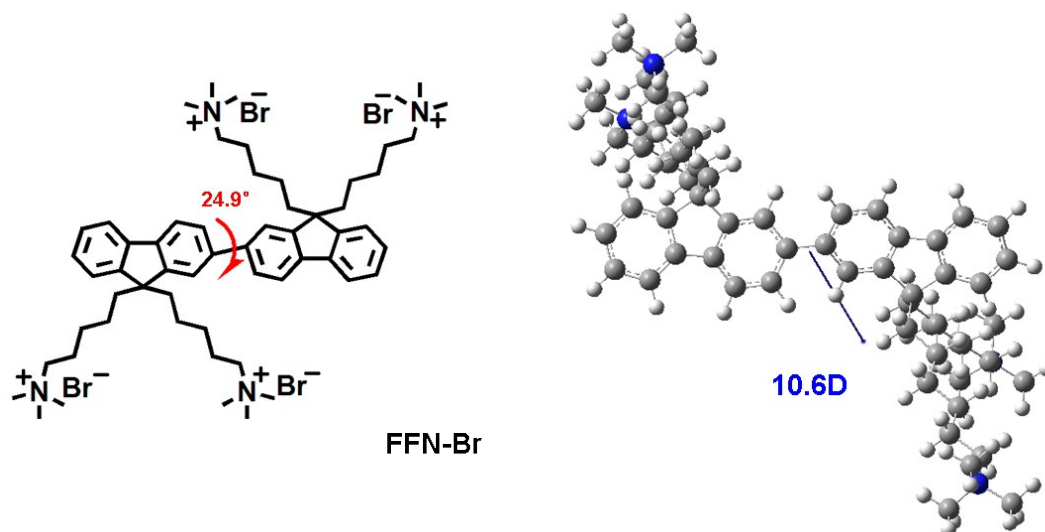


Figure S5. The density functional theory calculated results of the FFN-Br

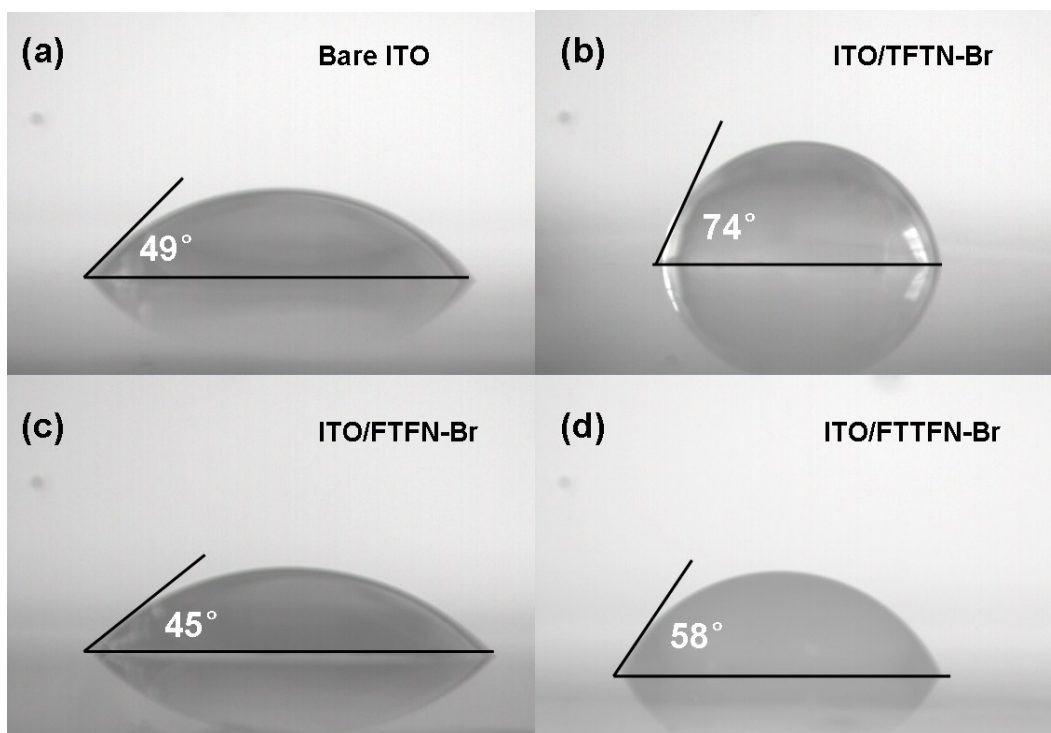


Figure S6. Water contact angle images of (a) bare ITO, (b) ITO/TFTN-Br (c) ITO/FTFN-Br and (d) ITO/FTTFN-Br

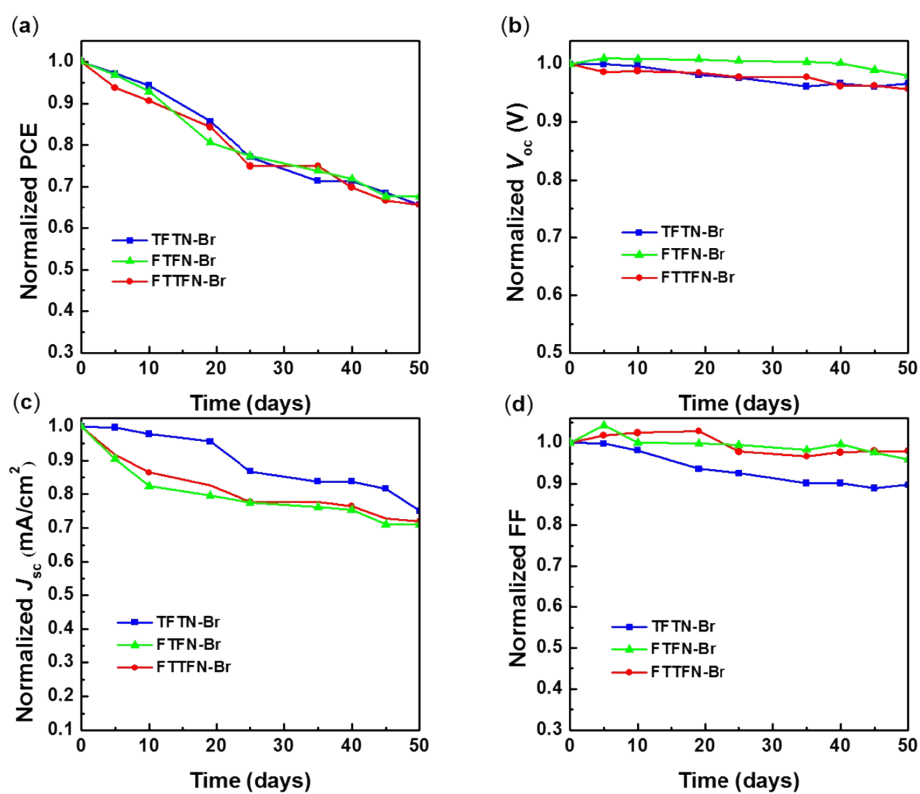


Figure S7. Stability test of the unencapsulated I-PSCs with various CSEs (a) PCE; (b) V_{oc} ; (c) J_{sc} ; (d) FF.

Reference

1. H. Wei, H. Zhang, H. Sun, W. Yu, Y. Liu, Z. Chen, L. Cui, W. Tian and B. Yang, *J. Mater. Chem.*, 2012, **22**, 17827-17832.
2. H. C. Chen, C. W. Lai, I. C. Wu, H. R. Pan, I. W. P. Chen, Y. K. Peng, C. L. Liu, C. h. Chen and P. T. Chou, *Adv. Mater.*, 2011, **23**, 5451-5455.