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 (δ=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 AlKa (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

\[ J = \frac{9\varepsilon_0\varepsilon_r\mu V^2}{8L^3} \]
Where $\varepsilon_0$ is the permittivity of free space ($8.85 \times 10^{-12}$ F·m$^{-1}$), $\varepsilon_r$ is the dielectric constant of P3HT or PCBM (assumed to 3), $\mu$ is the mobility of an electron, $V$ is the applied voltage, and $L$ is the film thickness. 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 Bu₄NPF₆ at a scan rate of 50 mV S⁻¹.
**Table S1.** Optical and electrochemical properties of the SMEs

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