Supporting Information

Effect of Organic Cathode Interfacial Layer on Efficiency and Stability Improvement of Polymer Solar Cells

Mingguang Li†, Wen Zhang†, Honglei Wang, Lingfeng Chen, Chao Zheng, and Runfeng Chen*

Key Laboratory for Organic Electronics and Information Displays & Institute of Advanced Materials, Jiangsu National Synergetic Innovation Center for Advanced Materials, Nanjing University of Posts and Telecommunications, Wenyuan Road, Nanjing, 210023, P.R. China.

† These authors contributed equally to this work.

Supporting methods

Fabrication of electron-only device. The structure of electron-only device was ITO/LiF/PTB7:PC71BM/CILs/Al. The preparation of active layer and the deposition of various CILs are identical to those adopted in the fabrication of PSCs. Therefore, the electron mobility can be extracted by fitting the current density-voltage curve using the field-dependent space charge limited current (SCLC) model of Mott-Gurney in the following equation1, 2:

\[
J = \frac{9}{8} \varepsilon \varepsilon_0 \mu e V^2 L^3 \exp\left[0.89 \left(\frac{V}{E_0 L}\right)^{0.5}\right]
\]

where \(\varepsilon\) is the dielectric constant of the blend film (\(\varepsilon=3\)), \(\varepsilon_0=8.85419 \times 10^{-12} \text{ C V}^{-1} \text{ m}^{-1}\), \(\mu_e\) is the zero-field electron mobility and \(L\) is the thickness of the films (100 nm). The calculated results of electron mobilities of these different organic CIL materials were shown in Fig. S5.
Supporting Figure

Fig. S1 Photograph of the PSC on ITO glass substrate

Fig. S2 UV-vis absorption spectra of PTB7:PC71BM blend film with LiF, BCP, Alq₃ and TmPyPB CILs.
Fig. S3  AFM height image (10.0 μm × 10.0 μm) of spin-coated PTB7:PC$_71$BM blend film

Fig. S4 (a) AFM height image (10.0 μm × 10.0 μm) of vacuum deposited TmPyPB CIL on spin-coated PTB7:PC$_71$BM blend film and (b) the magnified AFM image (2.0 μm × 2.0 μm)
Fig. S5 Current density-voltage curves of the electron-only devices based on PTB7:PC71BM with different CILs using LiF, BCP, Alq3, TmPyPB, and TmPyPB+LiF. Inset is the list of the corresponding electron mobility ($\mu_e$) measured by using SCLC model.
Fig. S6 (a) Current-voltage (J-V) curves and (b) Photo-stability characteristics of P3HT:PC_{61}BM-based PSCs using different CILs under ambient environment.

Table S1. LUMO, HOMO, bandgap (E_g), electron mobility (\(\mu_e\)) of the organic CIL materials

<table>
<thead>
<tr>
<th>CIL materials</th>
<th>LUMO (eV)</th>
<th>HOMO (eV)</th>
<th>(E_g) (eV)</th>
<th>(\mu_e) (cm^2V^{-1}s^{-1})</th>
<th>Reference</th>
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<tbody>
<tr>
<td>BCP</td>
<td>-3.0</td>
<td>-6.5</td>
<td>3.5</td>
<td>10^{-3}-10^{-6}</td>
<td>3-6</td>
</tr>
<tr>
<td>Alq_3</td>
<td>-3.1</td>
<td>-5.8</td>
<td>2.7</td>
<td>~10^{-5}</td>
<td>7, 8</td>
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<tr>
<td>TmPyPB</td>
<td>-2.7</td>
<td>-6.7</td>
<td>4.0</td>
<td>1\times10^{-3}</td>
<td>4, 9</td>
</tr>
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</table>
Reference