

Supporting Information

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

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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 equation^{1, 2}:

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

where ε is the dielectric constant of the blend film ($\varepsilon=3$), $\varepsilon_0=8.85419 \times 10^{-12} \text{ C V}^{-1}\text{m}^{-1}$, μ_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

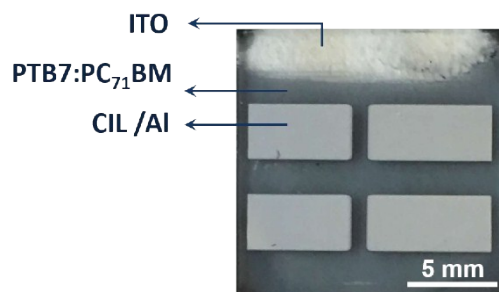


Fig. S1 Photograph of the PSC on ITO glass substrate

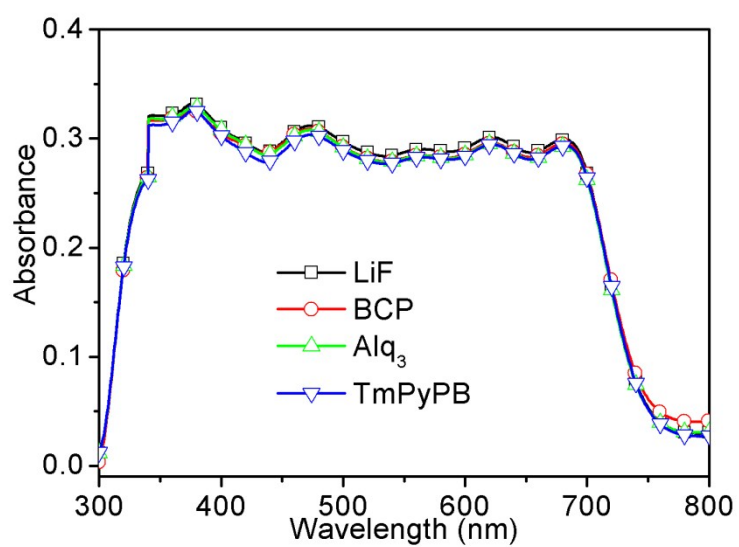


Fig. S2 UV-vis absorption spectra of PTB7:PC₇₁BM blend film with LiF, BCP, Alq₃ and TmPyPB CILs.

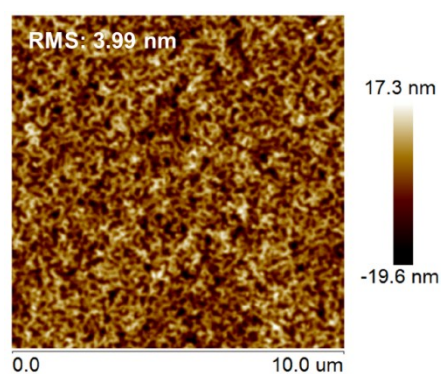


Fig. S3 AFM height image ($10.0\ \mu\text{m} \times 10.0\ \mu\text{m}$) of spin-coated PTB7:PC₇₁BM blend film

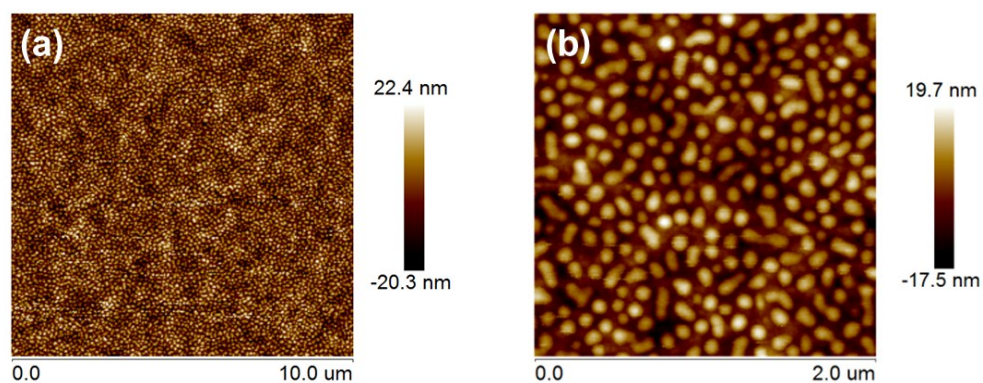


Fig. S4 (a) AFM height image ($10.0\ \mu\text{m} \times 10.0\ \mu\text{m}$) of vacuum deposited TmPyPB CIL on spin-coated PTB7:PC₇₁BM blend film and (b) the magnified AFM image ($2.0\ \mu\text{m} \times 2.0\ \mu\text{m}$)

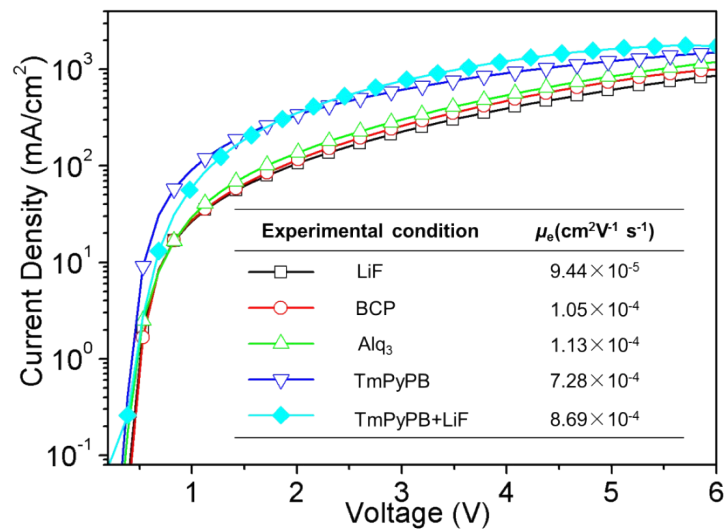


Fig. S5 Current density-voltage curves of the electron-only devices based on PTB7:PC₇₁BM with different CILs using LiF, BCP, Alq₃, TmPyPB, and TmPyPB+LiF. Inset is the list of the corresponding electron mobility (μ_e) measured by using SCLC model.

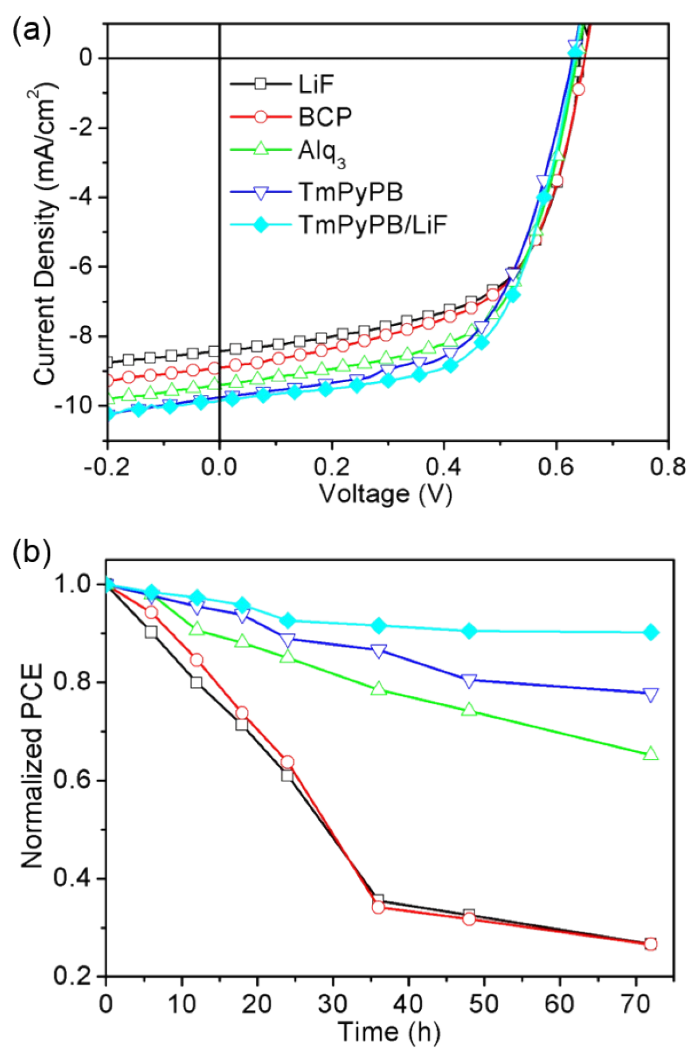


Fig. S6 (a) Current-voltage (J - V) curves and (b) Photo-stability characteristics of P3HT:PC₆₁BM-based PSCs using different CILs under ambient environment.

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

CIL materials	LUMO (eV)	HOMO (eV)	E_g (eV)	μ_e (cm ² V ⁻¹ s ⁻¹)	Reference
BCP	-3.0	-6.5	3.5	10 ⁻³ -10 ⁻⁶	3-6
Alq ₃	-3.1	-5.8	2.7	~10 ⁻⁵	7, 8
TmPyPB	-2.7	-6.7	4.0	1 × 10 ⁻³	4, 9

Reference

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