Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supplementary Information

Highly Efficient Polymer Solar Cells Based on a Universal Cathode Interlayer Composed of Metallophthalocyanine Derivative with Good Film-Forming Property

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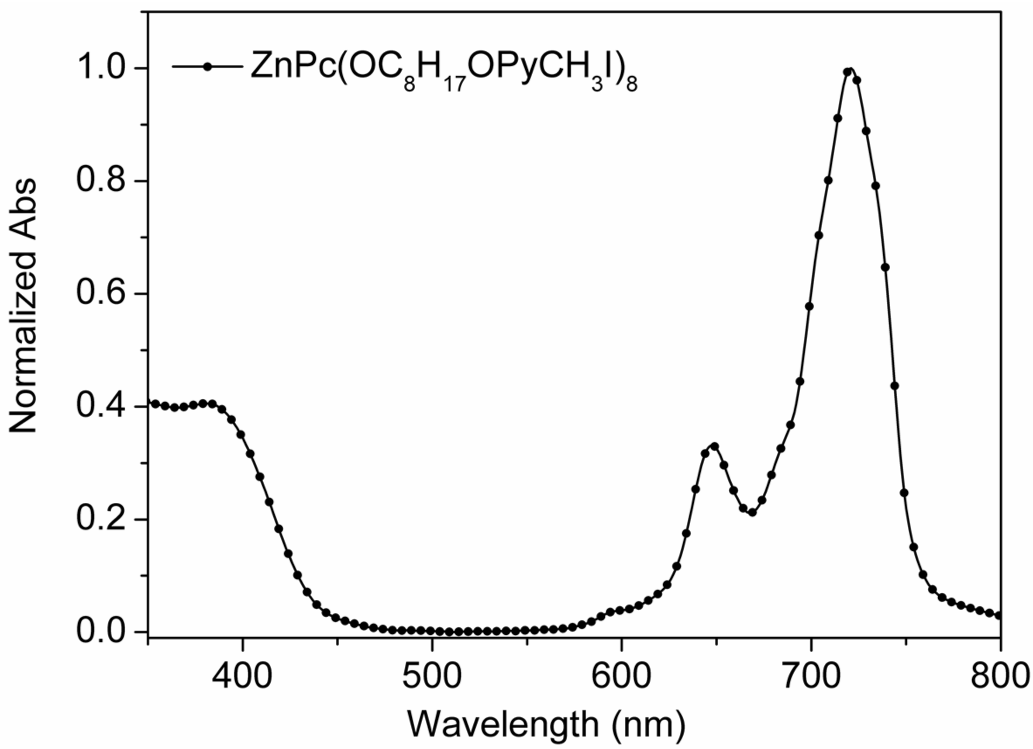

Figure S1. UV/Vis absorption spectrum of $ZnPc(OC_8H_{17}OPyCH_3I)_8$ in DMF.

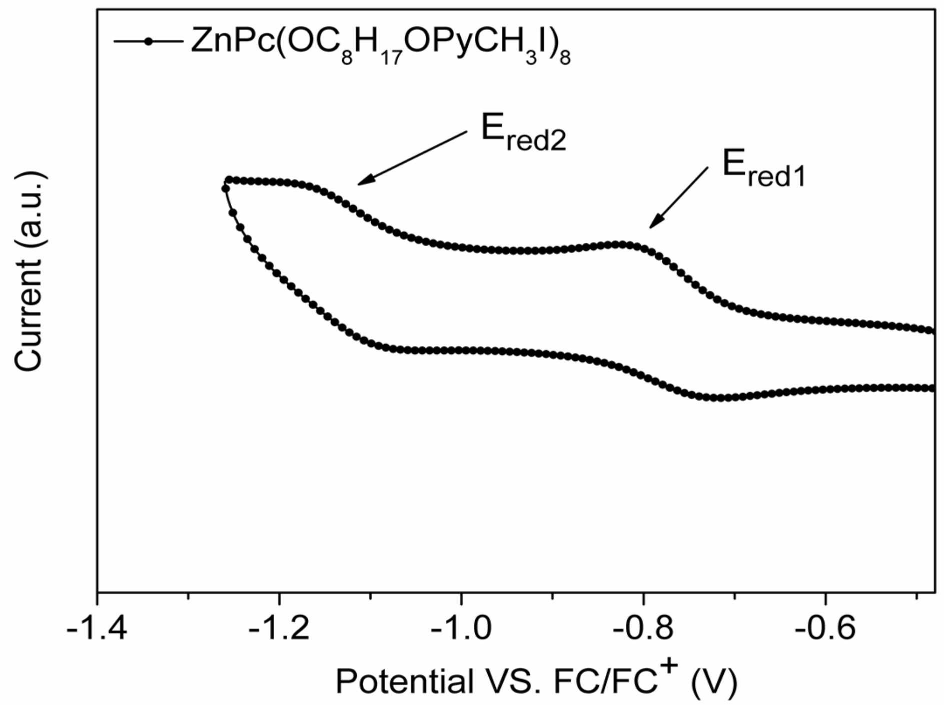

Figure S2. Cyclic voltammograms of $ZnPc(OC_8H_{17}OPyCH_3I)_8$ at room temperature, 0.1 M TBAPF6 in DMF (negative).

Table S1. Redox properties of $ZnPc(OC_8H_{17}OPyCH_3I)_8$ (vs. *FC*/*FC*$^+$).

E_{ox} (eV)	E_{red1} (V)	E_{red2} (V)	HOMO[a] (eV)	LUMO[b] (eV)	$E_g^{opt[c]}$ (eV)
-	-0.75	-1.12	-5.37	-4.05	1.32

[a] HOMO energy level was calculated using LUMO and E_g^{opt}.
[b] LUMO energy level was calculated using the reduction onset potential measured in DMF. The energy level of the ferrocene (Fc) reference (4.8 eV) was calibrated by measuring the cyclic voltammogram of Fc in corresponding solution.
[c] The optical band gap was calculated using the equation $E_g^{opt} = 1240 \times \lambda_{edge}^{-1}$, where λ_{edge} is the onset value of the absorption spectrum of the DMF solution in the direction of longer wavelength.

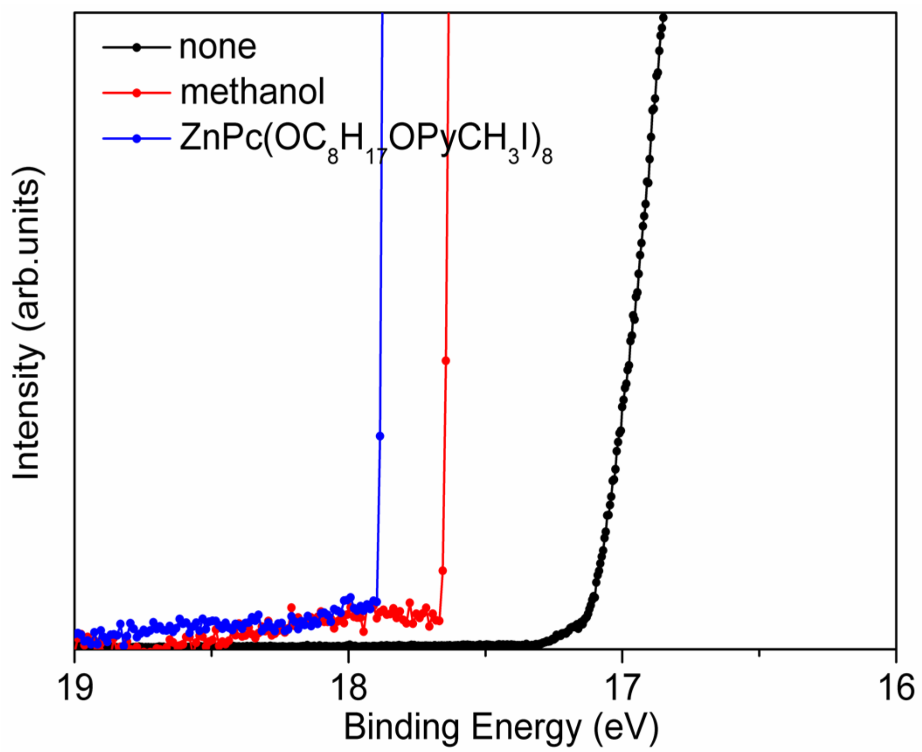

Figure S3. Ultraviolet photoelectron spectra of bare Al (black line), Al treated by methanol (red line) and Al covered by ~5nm $ZnPc(OC_8H_{17}OPyCH_3I)_8$ within the range of 16 – 19 eV.

Space charge limited current (SCLC) measurements of carrier-only devices

In order to obtain the electron and hole mobilities in the polymer solar cells, we carried out SCLC measurements of electron-only and hole-only devices. Charge carrier mobility can be measured in the SCLC regime as described by

$$J=9\varepsilon_0\varepsilon_r\mu V^2/8L^3, \qquad (1)$$

Where ε_0 is the permittivity of free space (8.8542×10^{-12} F/m), ε_r is the dielectric constant of the active layer, μ_e is the electron mobility, V is the voltage drop across the device, L is the active layer thickness. The above equation holds if the mobility is field independent. ε_r is assumed to be 3.9 and L is 120nm in our analysis. Figure S4a and S4b present our $J^{0.5}$-V analysis for the electron-only and hole-only devices, where V_r (the voltage drop due to contact resistance and series resistance across the electrodes) and V_{bi} (the built-in voltage due to the difference in work function of the two electrodes at both sides of active layer) are subtracted from experimental applied voltage. A straight line going through the origin of $J^{0.5}$-V curves for the devices signifies that the mobility is field independent at field up to 2×10^5 V/cm. The field independent mobilities calculated from Eq. (1) are presented in Table S2.

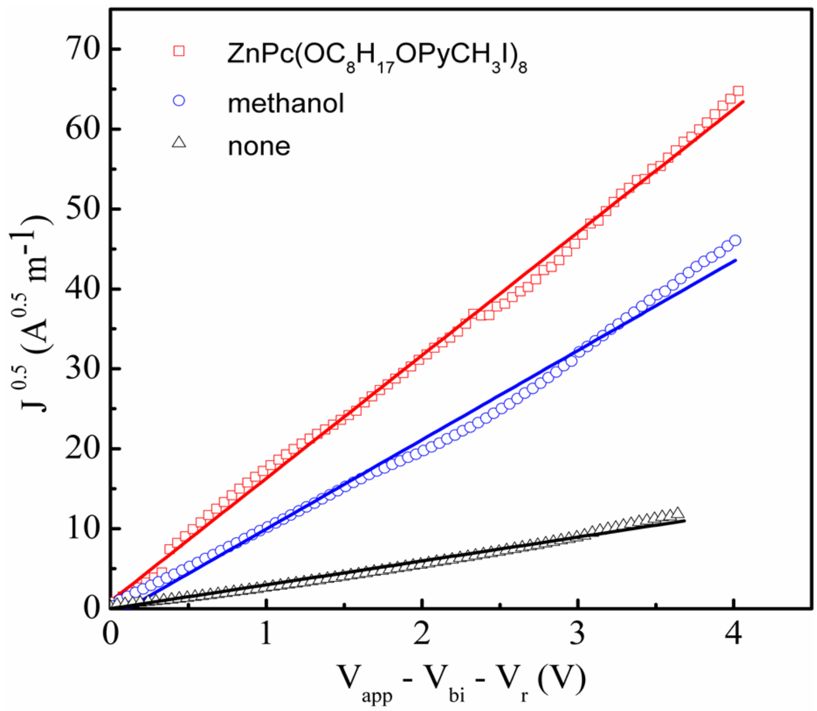

Figure S4a. $J^{0.5}$ vs. V_{appl}-V_{bi}-V_r plots for the electron-only devices.

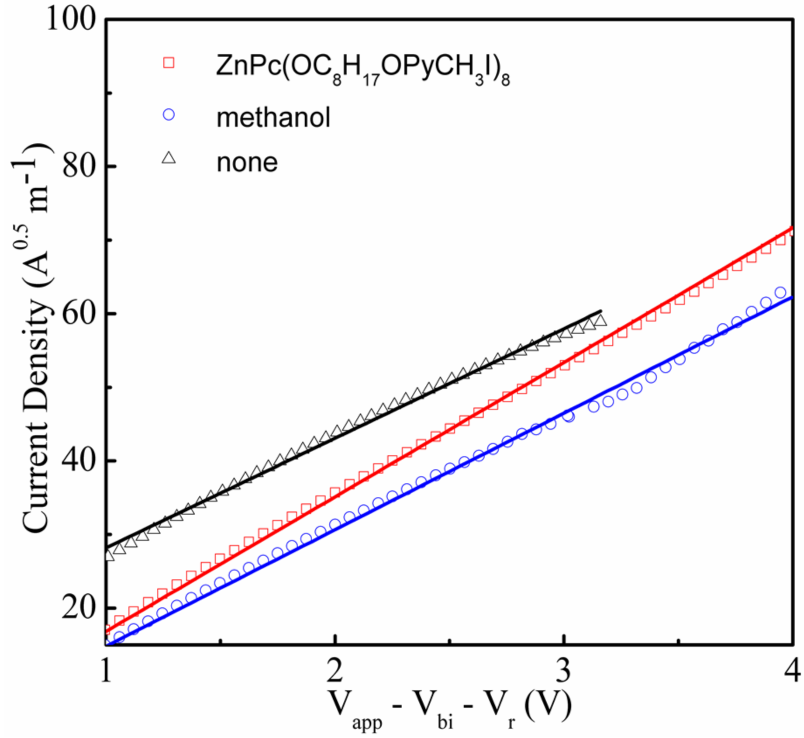

Figure S4b. $J^{0.5}$ vs. V_{appl}-V_{bi}-V_r plots for the hole-only devices.

Table S2. Electron and hole mobility of the devices with various interfacial treatments.

Active Layer Treatment	Electron-only devices	Hole-only devices
	Electron mobility [$cm^2 V^{-1} S^{-1}$]	Hole mobility [$cm^2 V^{-1} S^{-1}$]
None	1.34×10^{-5}	3.25×10^{-4}
Methanol	1.82×10^{-4}	3.95×10^{-4}
$ZnPc(OC_8H_{17}OPyCH_3I)_8$	3.29×10^{-4}	4.12×10^{-4}

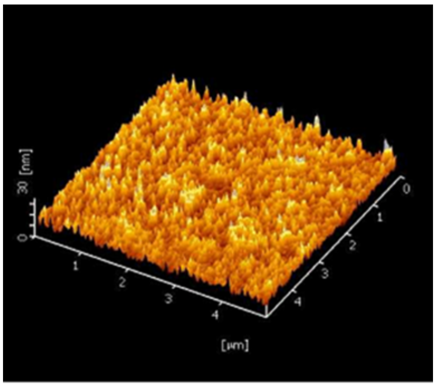

Figure S5. AFM image of PFN on PTB7:$PC_{71}BM$ film.

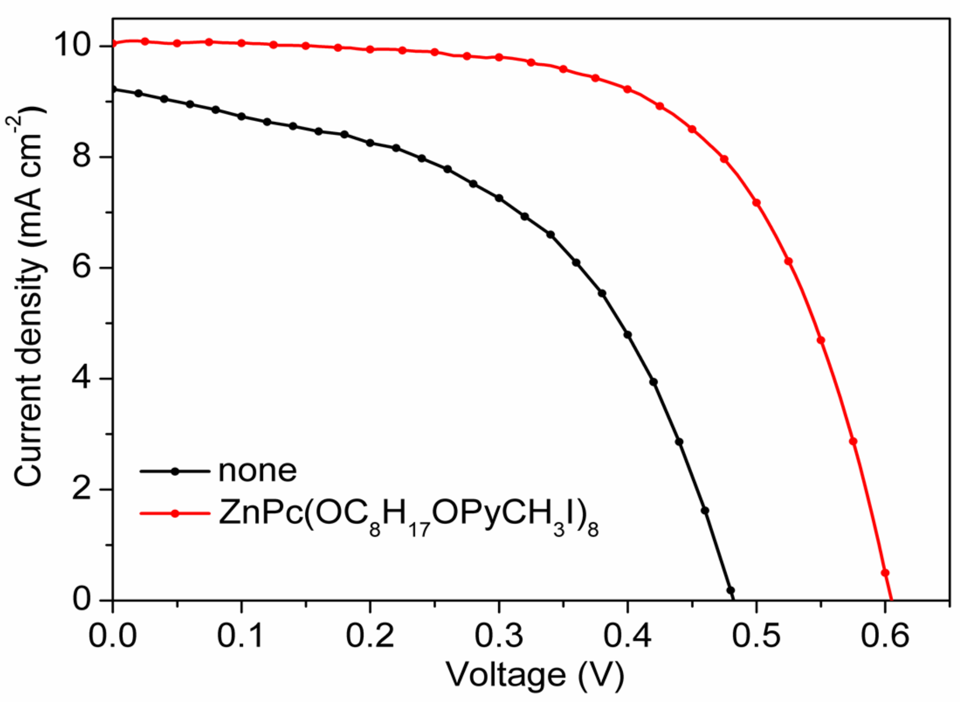

Figure S6. Current density versus voltage (*J*–*V*) characteristics of the PSCs based on P3HT:$PC_{61}BM$ with (red line) and without (black line) $ZnPc(OC_8H_{17}OPyCH_3I)_8$ as a CIL.

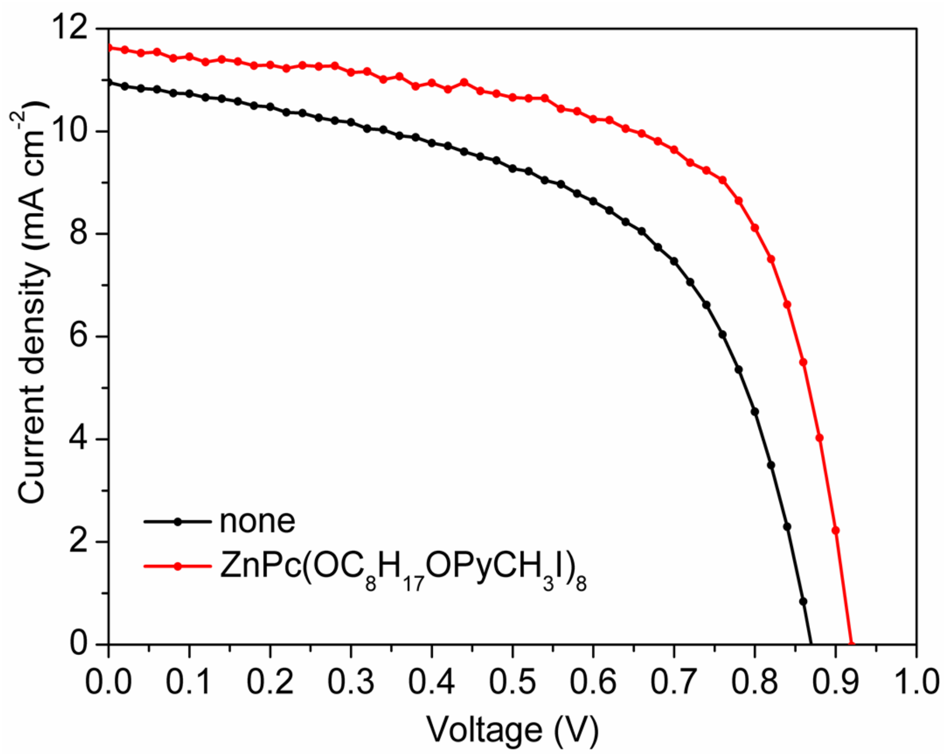

Figure S7. Current density versus voltage (*J–V*) characteristics of the PSCs based on PCDTBT:$PC_{71}BM$ with (red line) and without (black line) $ZnPc(OC_8H_{17}OPyCH_3I)_8$ as a CIL.

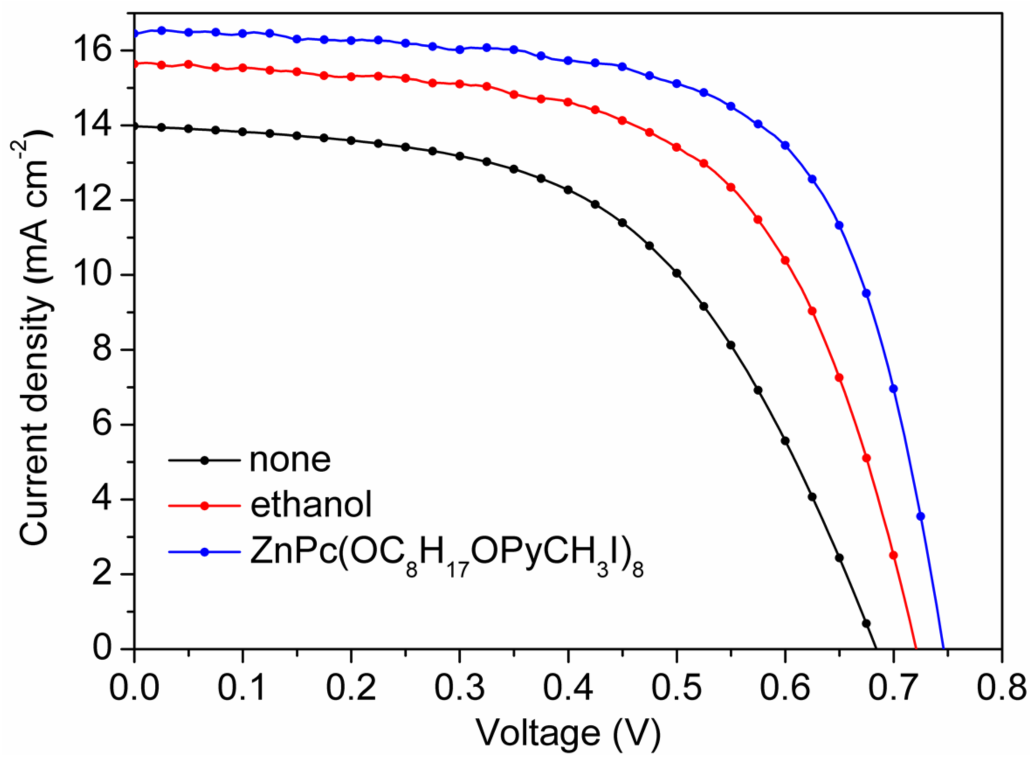

Figure S8. Current density versus voltage (*J–V*) characteristics of devices with $ZnPc(OC_8H_{17}OPyCH_3I)_8$ (blue line) as a CIL, with (red line) and without (black line) alcohol treatment at the surface of PTB7:$PC_{71}BM$ under 100 mW cm^{-2} AM 1.5G illumination.