

Electronic Supplemental Information for

Ethanolamine-functionalized fullerene as an efficient electron transport layer for high-efficiency inverted polymer solar cells

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S1. FTIR spectra of C₆₀-ETA and ETA.

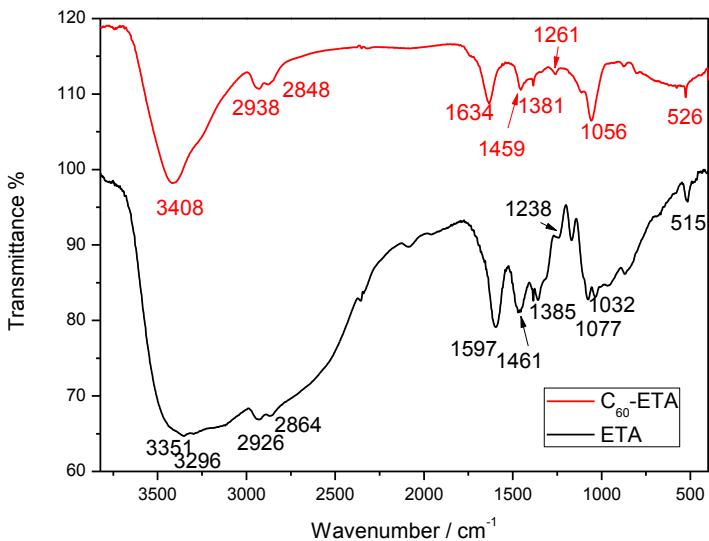


Figure S1. FTIR spectra of C₆₀-ETA and ETA.

S2. XPS analysis of C₆₀-ETA.

Table S1. The binding energies (BE) of C1s, N1s and O1s cores and calculated atomic percentage (Atom%) of C, N, O.

Core	Start BE (eV)	Peak BE (eV)	End BE (eV)	FWHM ^[a] (eV)	Area ^[b]	Atom% ^[c]	Atomic ratio ^[d]	Theor. Atomic ratio ^[e]
C1s	291.25	284.5	281.6	1.44	65402.24	78.17		
N1s	403.05	398.52	395.8	1.46	10982.78	8.10	9.65:1:1.7	9.5:1:1
O1s	535	531.65	527.5	1.72	27864.92	13.73		

^[a] FWHM: full width at half maximum; ^[b] Integrated area; ^[c] Calculated from the percentage of the integrated area; ^[d] The atomic ratio of C:N:O; ^[d] Theoretical atomic ratio of C:N:O calculated according to the estimated average molecular formula of C₆₀(NHC₂H₄OH)₈(H)₈ (=C₇₆N₈O₈H₅₆). The deviation of atomic ratio of N:O is likely because of the well-known inaccuracy of O1s signal intensity measured by XPS. Note that the atomic ratio of C:N calculated from elemental analysis is ~9.44:1 according to the weight percentages of 78.43% and 9.69% for C and N, agreeing with those of the calculated one and measured by XPS.

S3. TGA analysis of C₆₀-ETA.

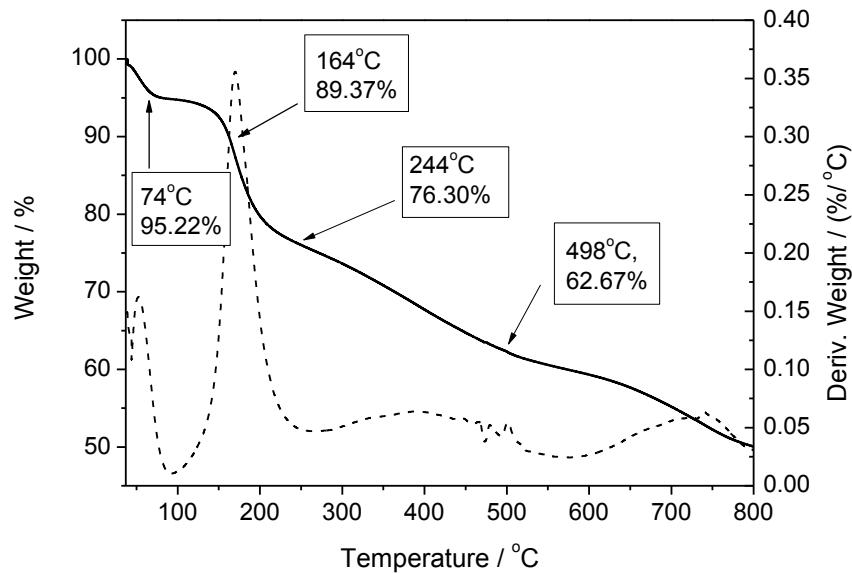


Figure S2. TGA curve (solid line) and differential thermo-gravimetric (DTG) curve (dashed line) of C₆₀-ETA.

S4. Transmittance spectra of ITO and ITO/C₆₀-ETA

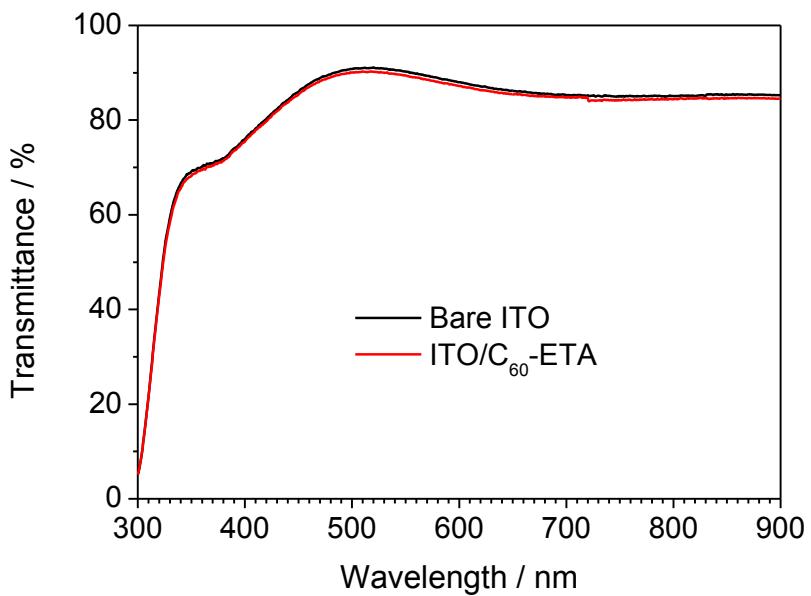


Figure S3. Transmittance spectra of bare ITO and ITO/C₆₀-ETA.

S5. AFM height images of ITO with C₆₀-ETA or ZnO layer.

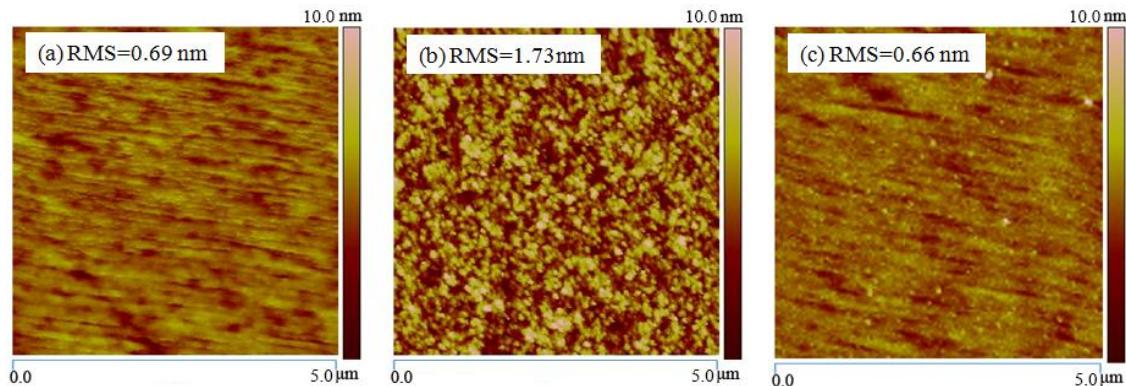


Figure S4. AFM height images ($5 \mu\text{m} \times 5 \mu\text{m}$) of bare ITO (a), ITO/ZnO (b), ITO/C₆₀-ETA (c).

S6. Enhancement ratios of the photovoltaic parameters.

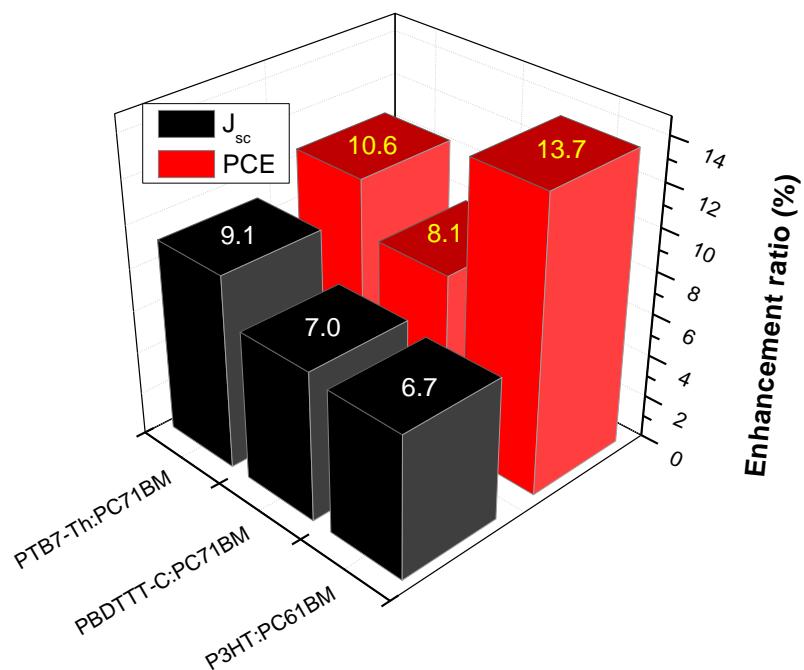


Figure S5. Enhancement ratios of J_{sc} and PCE for the C₆₀-ETA-incorporated devices relative to those of ZnO-incorporated ones.

S7. UV-vis absorption spectra of different active layers on ITO/C₆₀-ETA or ITO/ZnO.

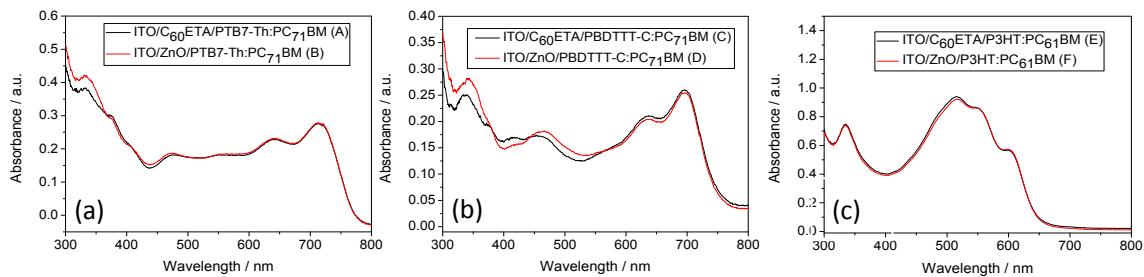


Figure S6. UV-vis absorption spectra of PTB7-Th:PC₇₁BM (a), PBDTTT-C:PC₇₁BM (b) and P3HT:PC₆₁BM (c) active layer films on ITO/C₆₀-ETA or ITO/ZnO.

S8. Electron mobilities of different active layer films on ITO/C₆₀-ETA or ITO/ZnO.

Table S2. Electron mobilities of different active layer films on ITO/C₆₀-ETA or ITO/ZnO.

Active layer	Device	ETL	μ_e (cm ² V ⁻¹ s ⁻¹) ^[a]
PTB7-Th:PC ₇₁ BM	A	C ₆₀ -ETA	5.54×10^{-4}
	B	ZnO	1.51×10^{-4}
PBDTTT-C:PC ₇₁ BM	C	C ₆₀ -ETA	4.19×10^{-4}
	D	ZnO	1.58×10^{-4}
P3HT:PC ₆₁ BM	E	C ₆₀ -ETA	9.60×10^{-4}
	F	ZnO	1.27×10^{-4}

^[a] Measured by electron-only devices with the structure of ITO/ETL/active layer/Ca/Al.

S9. Determination of work function of ITO/C₆₀-ETA or ITO/ZnO by SKPM.

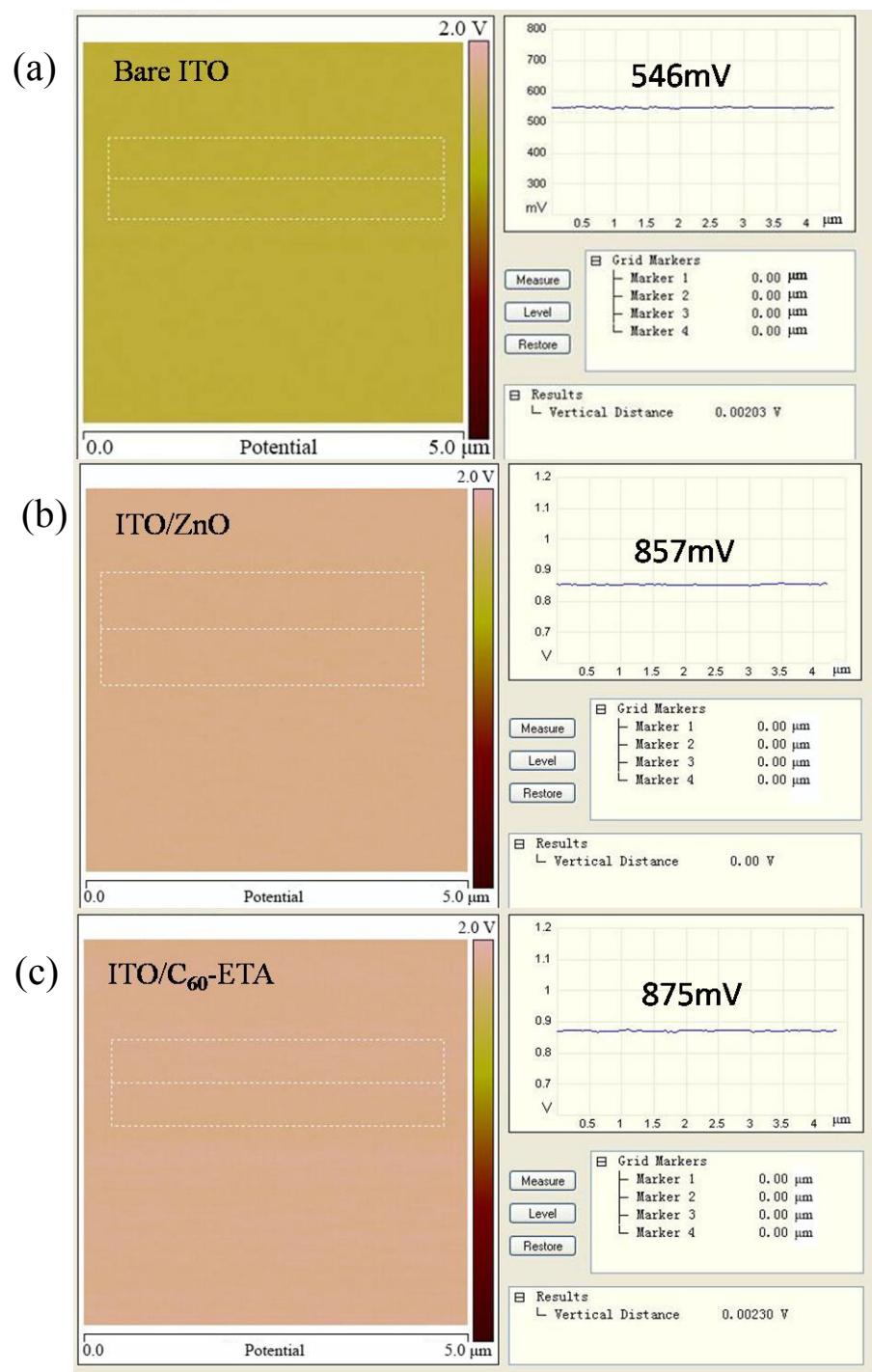


Figure S7. Surface potential images ($5 \mu\text{m} \times 5 \mu\text{m}$) and the surface potentials of bare ITO (a), ITO/ZnO (b) and ITO/C₆₀-ETA (c).

Table S3. The surface potentials and work functions of ETLs.

Device	ITO/ETL		
	without ETL (bare)	ZnO ETL	C ₆₀ -ETA ETL
Surface potential (SP, mV)	546	857	875
ΔSP (mV) ^a	-	311	329
ΔΦ (eV) ^b	-	0.31	0.33
Φ (eV)	-4.7 ^c	-4.39	-4.37

^a ΔSP is the surface potential change of ITO/ETL relative to the bare ITO;

^b Φ is the work function of film sample, ΔΦ is the work function change of ITO/ETL relative to the bare ITO. ΔΦ = eΔSP;

^c The work function of the bare ITO ($\Phi(\text{bare ITO}) = -4.7 \text{ eV}$) is referred to ref. S1.

$$\Phi(\text{ITO/ETL}) = \Phi(\text{bare ITO}) + \Delta\Phi.$$

Reference:

[S1]. Z. He, C. Zhong, S. Su, M. Xu, H. Wu, Y. Cao, *Nature Photon.* 2012, **6**, 593.