Supporting Information for

Amphiphilic Fullerenes/ZnO Hybrids as Cathode Buffer Layer to Improve Charge Selectivity of Inverted Polymer Solar Cells

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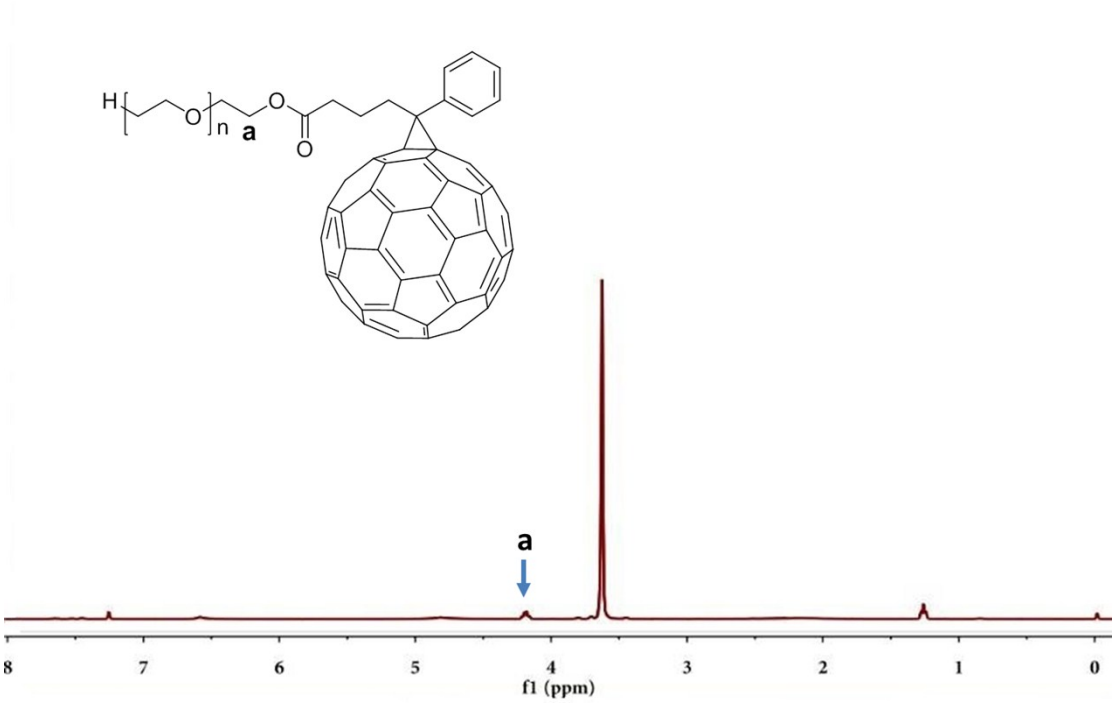


Figure S1.[1]HNMR spectrum of C60-PEG and the inset is the molecular structure of C60-PEG.

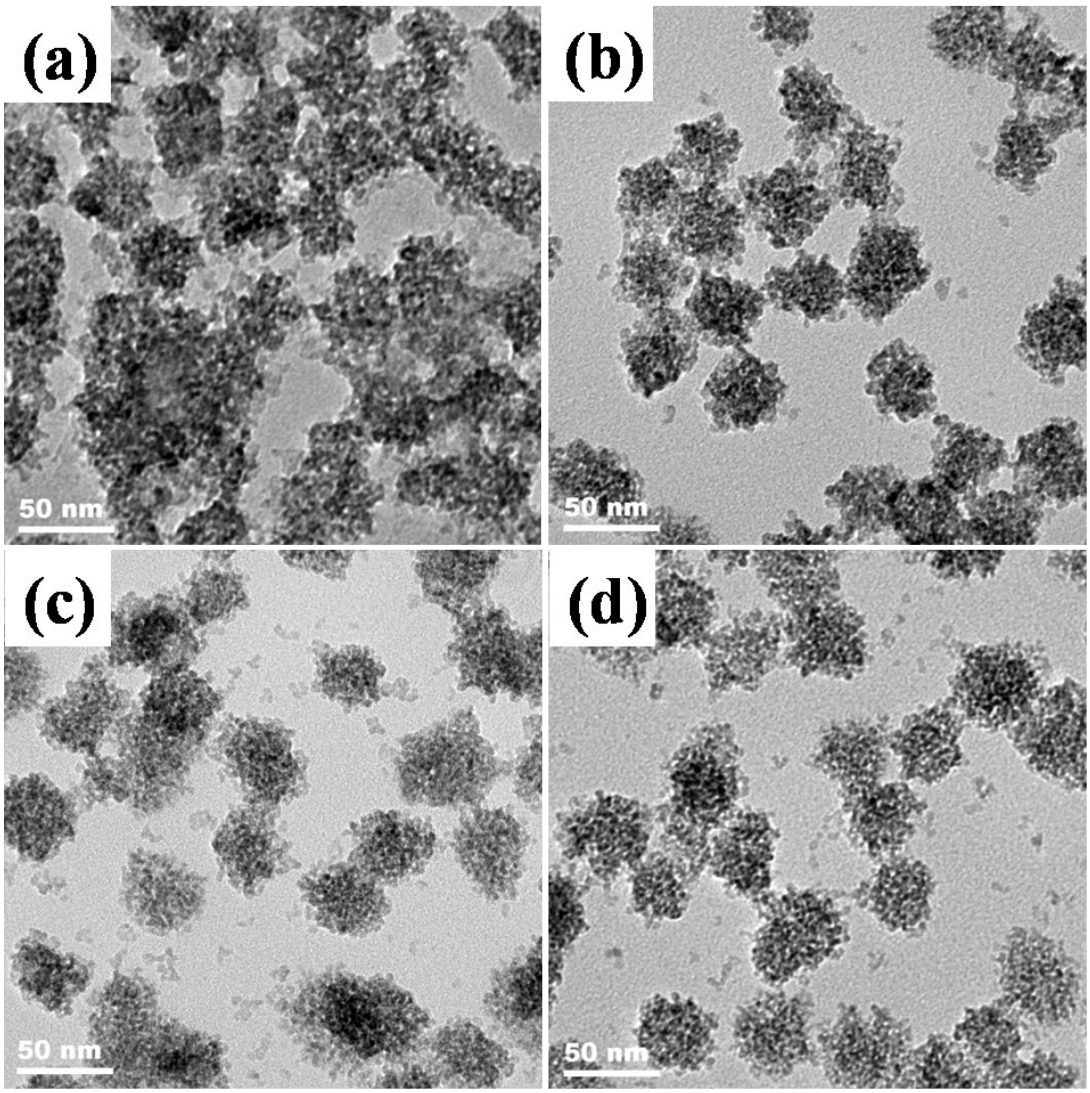


Figure S2. TEM images of (a) ZnO, (b) ZnO/1%C60-PEG, (c) ZnO/3%C60-PEG and (d) ZnO/5%C60-PEG.

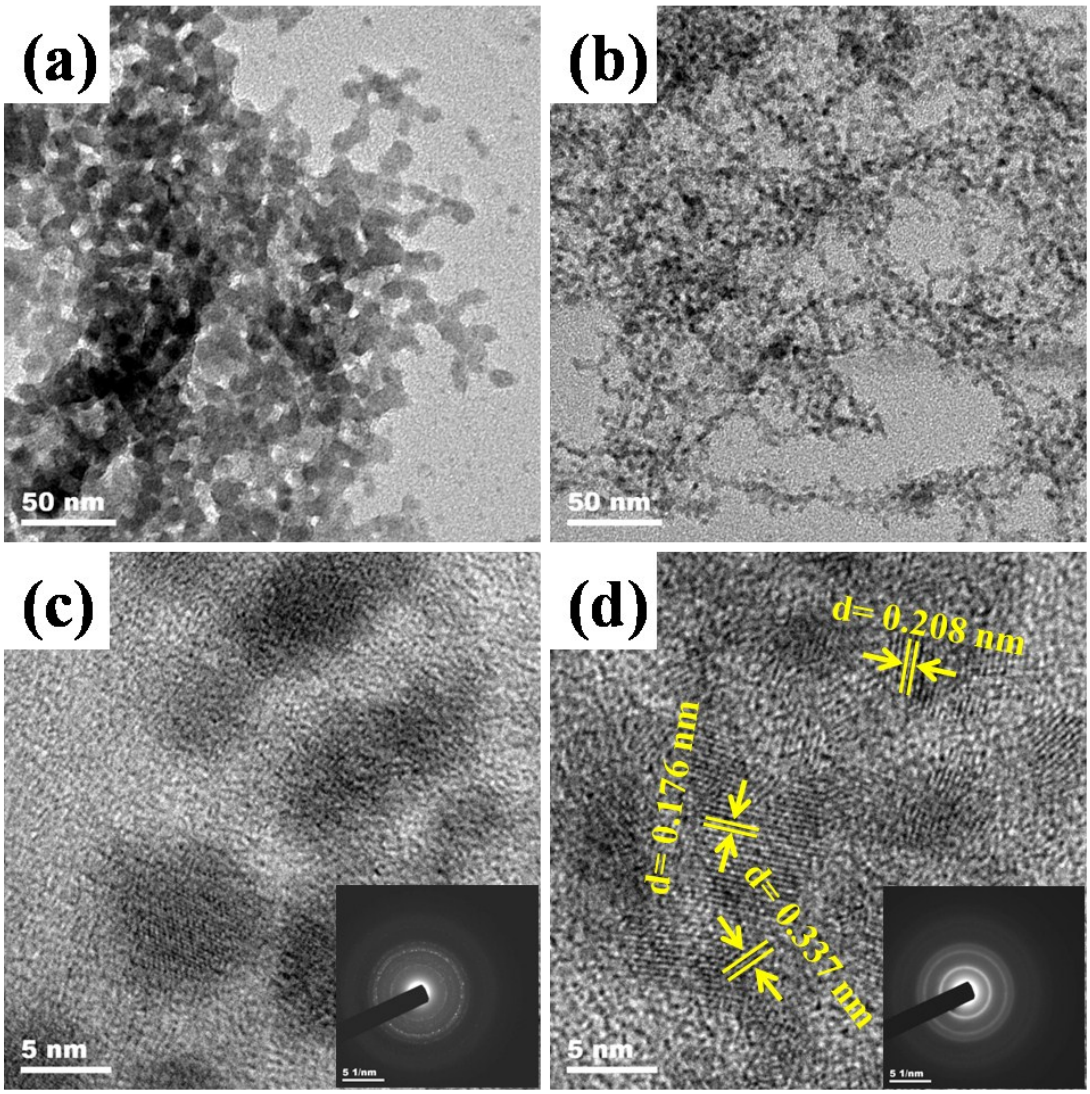
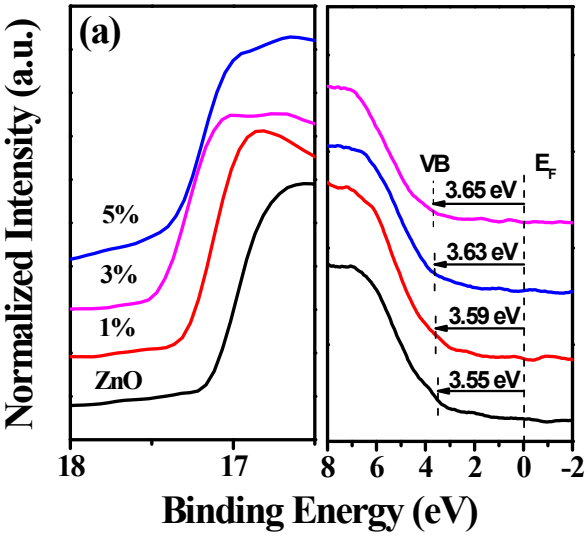
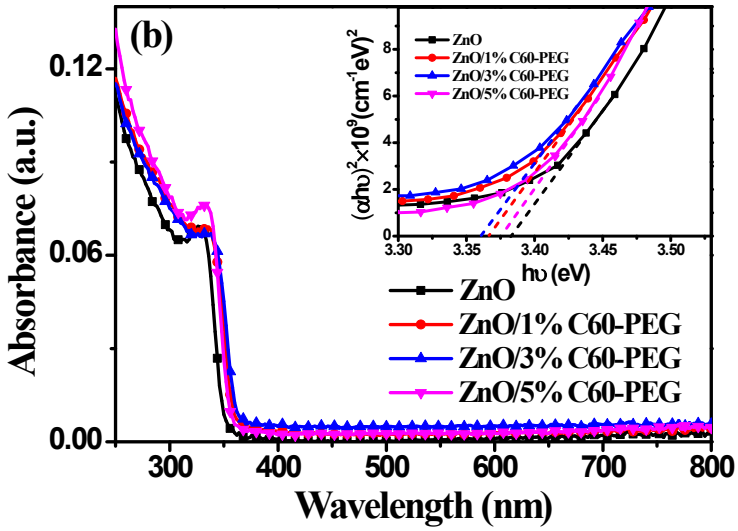


Figure S3. TEM images and the corresponding HRTEM images of (a, c) CdS and (b,d) CdS@3%C60-PEG. The inset of (c) and (d) is the SAED pattern of CdS and CdS@3%C60-PEG.


(a)
Normalized Intensity (a.u.)
5%
3%
1%
ZnO
VB
E_F
3.65 eV
3.63 eV
3.59 eV
3.55 eV
18
17
8
6
4
2
0
-2
Binding Energy (eV)


(b)
Absorbance (a.u.)
0.12
0.06
0.00
300
400
500
600
700
800
Wavelength (nm)
(αhυ)²×10⁹(cm⁻¹eV)²
hυ (eV)
ZnO
ZnO/1% C60-PEG
ZnO/3% C60-PEG
ZnO/5% C60-PEG

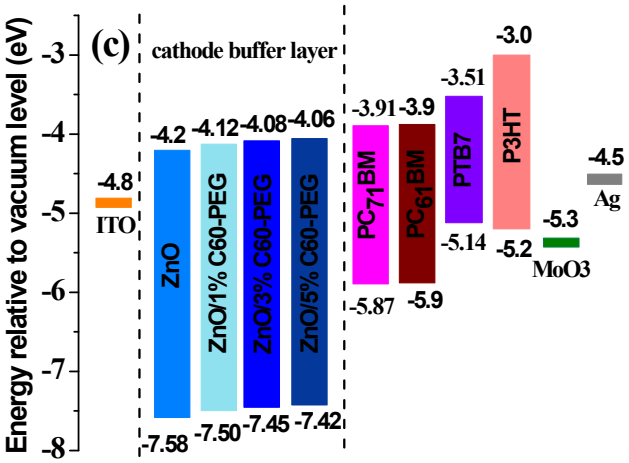


Figure S4. (a) UPS spectra and (b) UV–vis absorbance spectra (the inset is plots of $(\alpha hv)^2$ versus energy) of ZnO, ZnO/1%C60-PEG, ZnO/3%C60-PEG and ZnO/5%C60-PEG; (c) the corresponding energy level diagram of the components of the devices.

Table S1. Energy levels of ZnO, ZnO/1%C60-PEG, ZnO/3%C60-PEG and ZnO/5%C60-PEG.

Buffer layer	Eg(UV-Vis)	HOMO(UPS)	LUMO(Eg)
ZnO	3.38	7.58	4.20
ZnO/1% C60-PEG	3.38	7.50	4.12
ZnO/3% C60-PEG	3.37	7.45	4.08
ZnO/5% C60-PEG	3.36	7.42	4.06

Table S2. Electron mobility of (a)ZnO, (b) ZnO@0.1%C60-PEG, (c) ZnO@0.5%C60-PEG, (d) ZnO@1%C60-PEG, and (e) ZnO@5%C60-PEG.

Devices	a	b	c	**d**	e
μ_e ($cm^2\ V^{-1}s^{-1}$)	1.96×10^{-4}	4.36×10^{-4}	6.83×10^{-4}	$\mathbf{9.75\times10^{-4}}$	6.31×10^{-4}

Table S3. Electron mobility of (a)ZnO, (b) ZnO/1%C60-PEG, (c) ZnO/3%C60-PEG, and (d) ZnO/5%C60-PEG.

Devices	a	b	**c**	d
μ_e ($cm^2\ V^{-1}s^{-1}$)	2.45×10^{-4}	4.18×10^{-4}	$\mathbf{8.11\times10^{-4}}$	5.85×10^{-4}

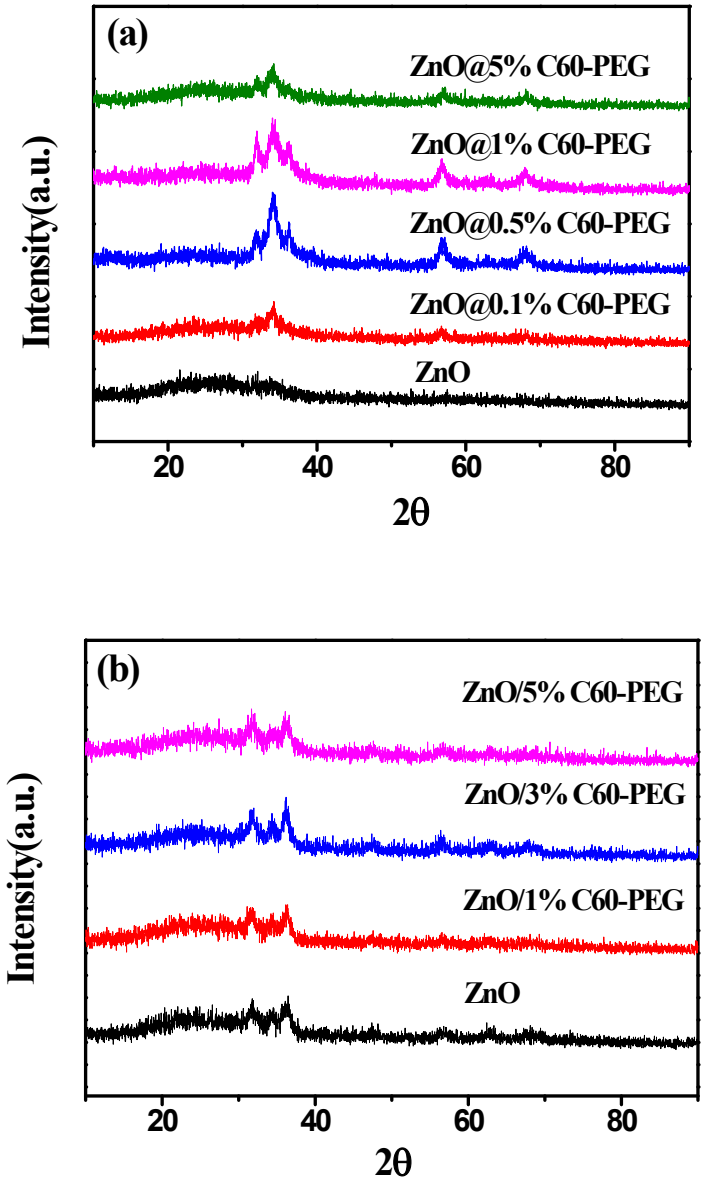


Figure S5. (a) XRD patterns of ZnO, ZnO@0.1%C60-PEG, ZnO@0.5%C60-PEG, ZnO@1%C60-PEG and ZnO@5%C60-PEG. (b) XRD patterns of ZnO, ZnO/1%C60-PEG, ZnO/3%C60-PEG and ZnO/5%C60-PEG.

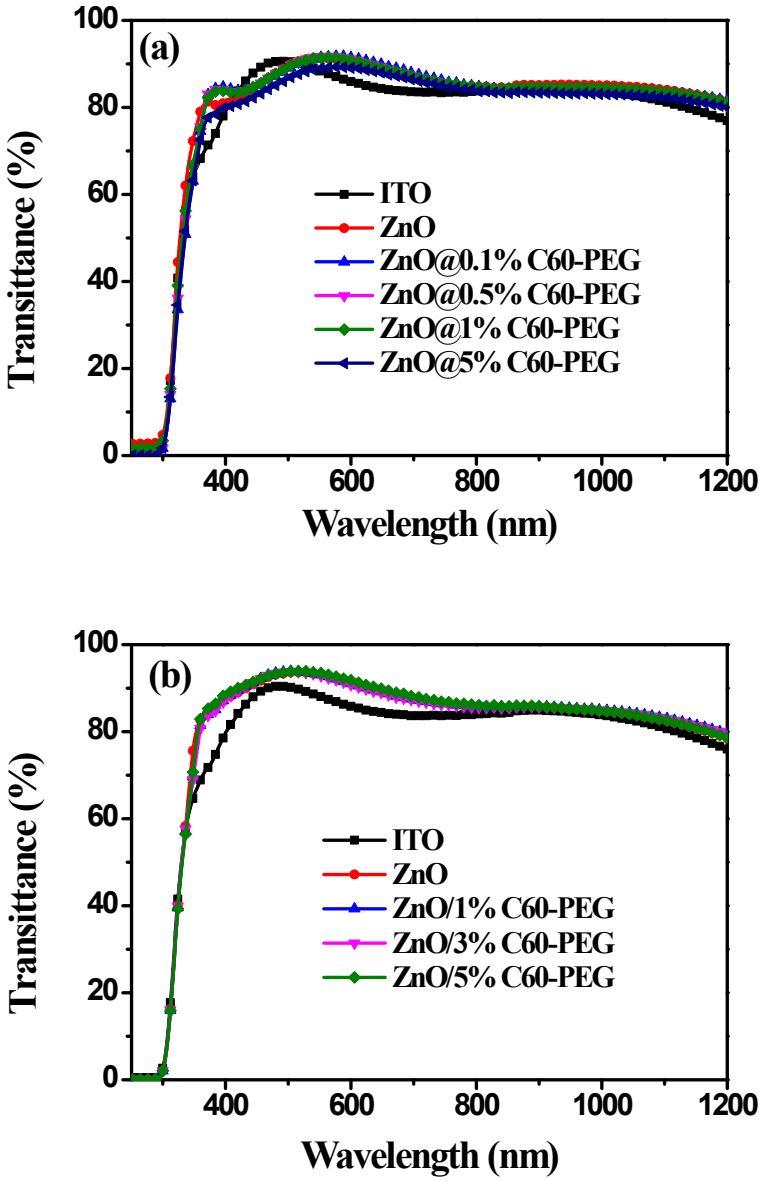


Figure S6. (a) Optical transmission spectra of ITO, ZnO, ZnO@0.1%C60-PEG, ZnO@0.5%C60-PEG, ZnO@1%C60-PEG and ZnO@5%C60-PEG. (b) Optical transmission spectra of ITO, ZnO, ZnO/1%C60-PEG, ZnO/3%C60-PEG and ZnO/5%C60-PEG.

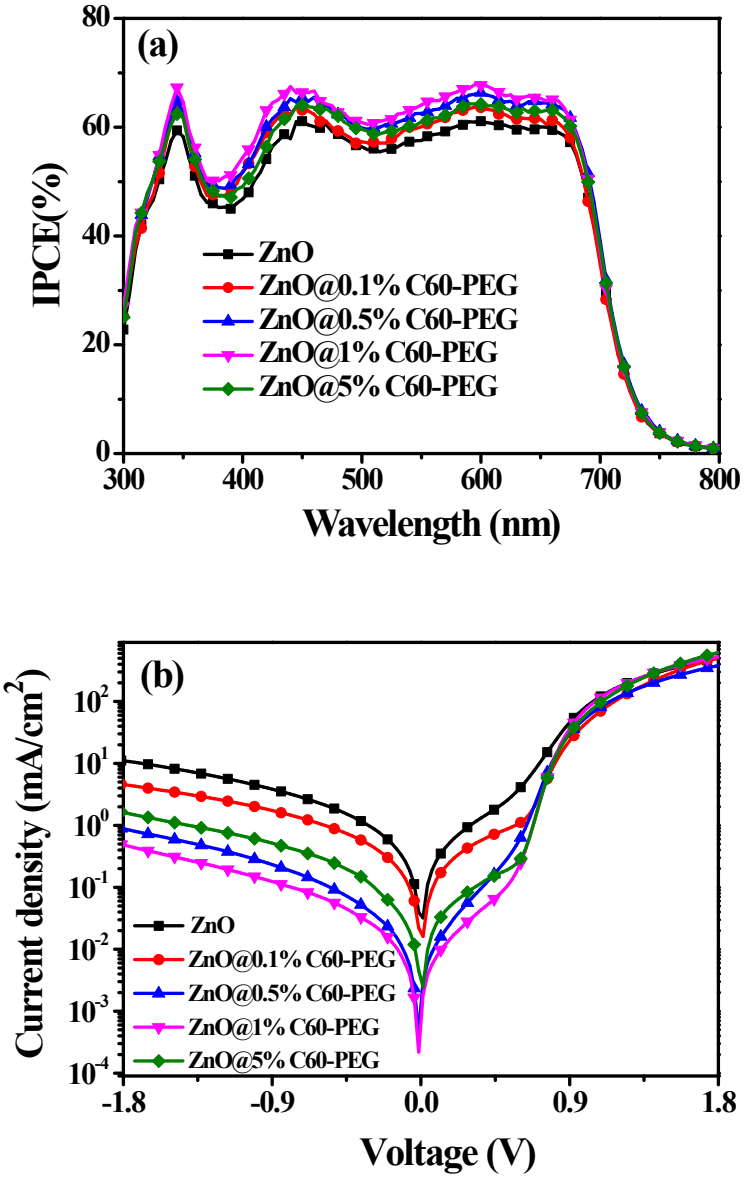


Figure S7. Performance of devices under simulated AM 1.5 G (100 mW·cm^{-2}) illumination. (a) IPCE spectra and (b) *J-V* curve under dark of the devices ITO/cathode buffer layer/PTB7:$PC_{71}BM$/MoO_3/Ag.

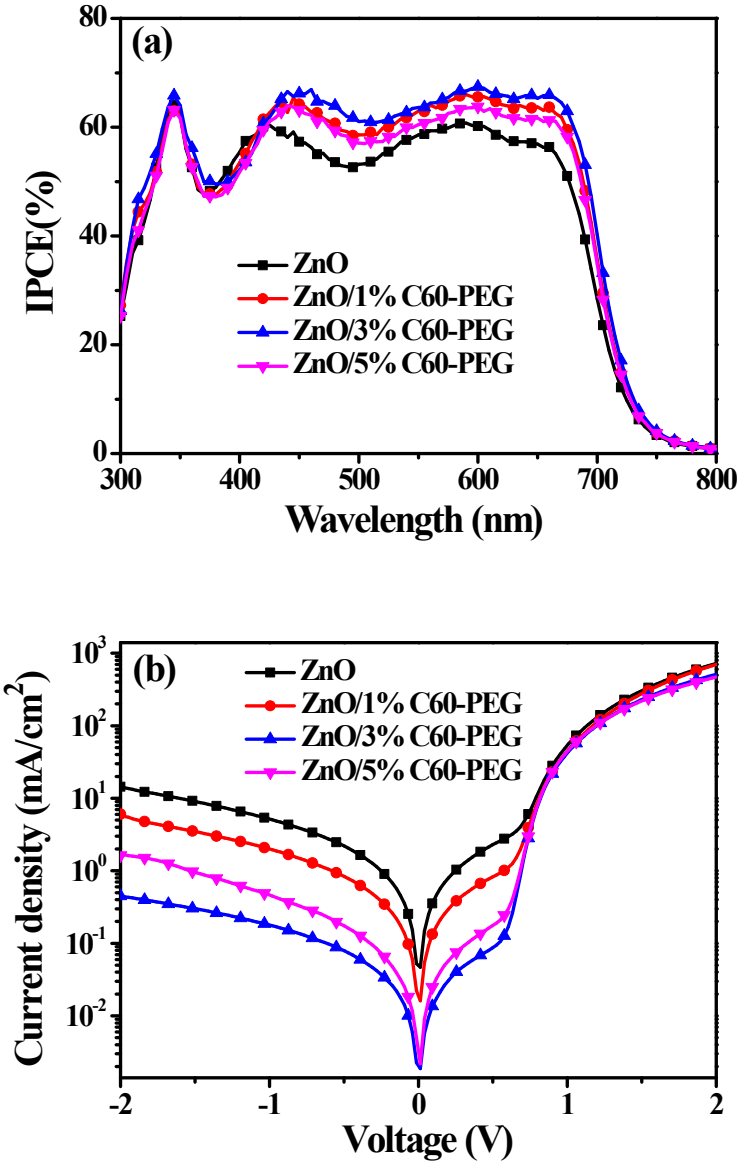


Figure S8. Performance of devices under simulated AM 1.5 G (100 mW·cm^{-2}) illumination. (a) IPCE spectra and (b) *J-V* curve under dark of the devices ITO/cathode buffer layer/PTB7:$PC_{71}BM$/MoO_3/Ag.

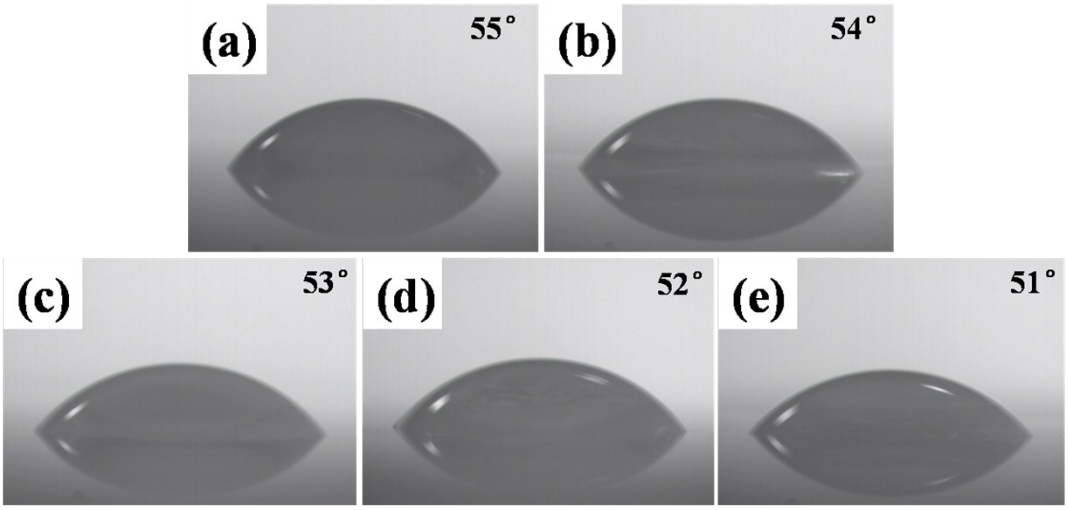


Figure S9. Measured water contact angle between a drop of deionized water on (a) ZnO, (b) ZnO@0.1%C60-PEG, (c) ZnO@0.5%C60-PEG, (d) ZnO@1%C60-PEG and (e) ZnO@5%C60-PEG.

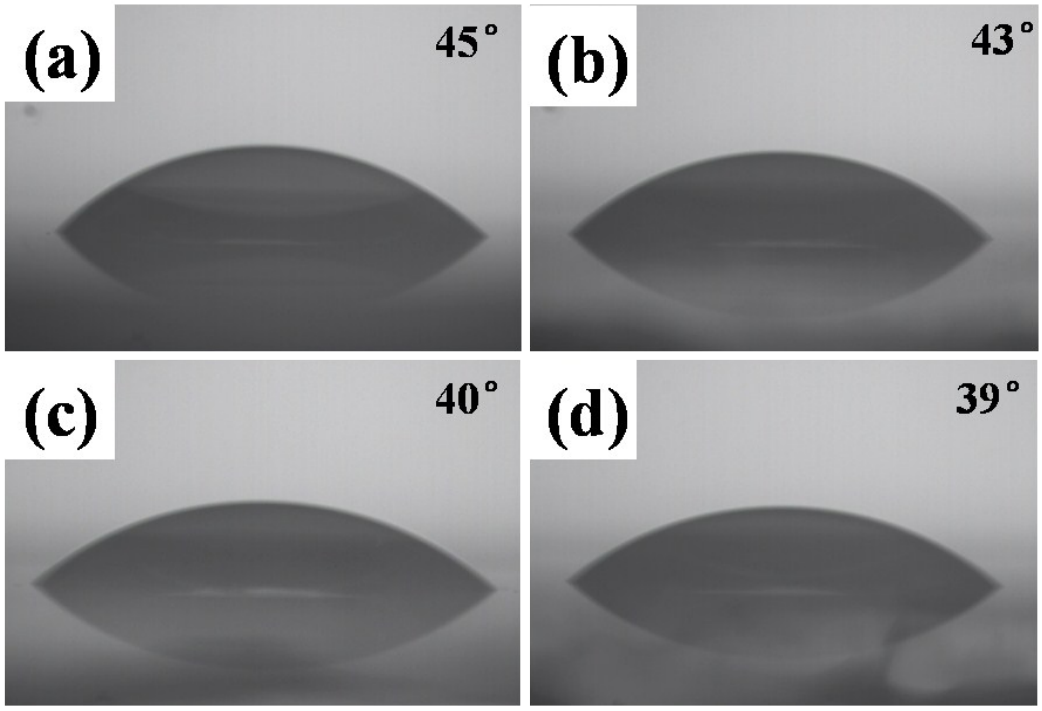
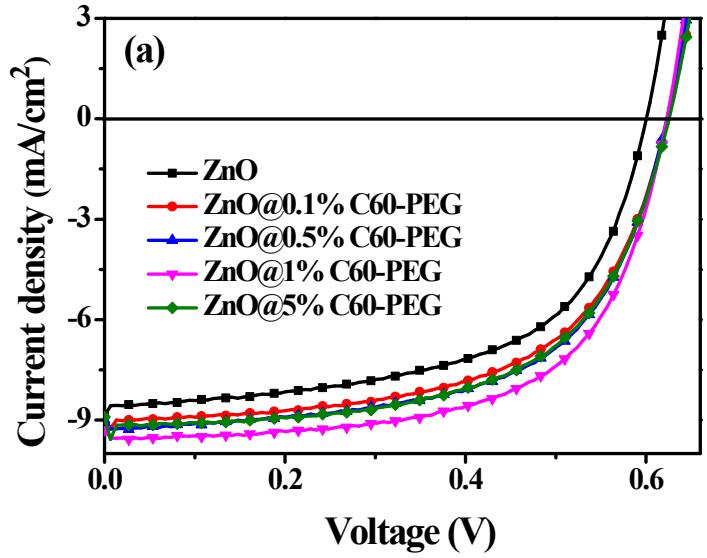
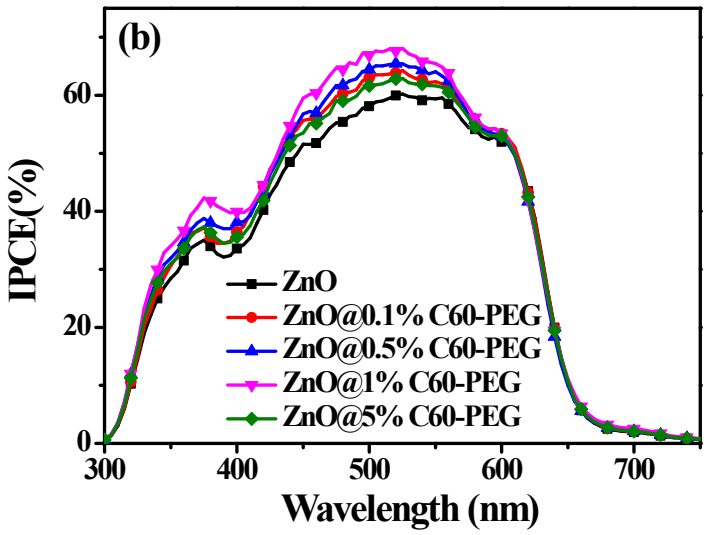


Figure S10. Measured water contact angle between a drop of deionized water on (a) ZnO, (b) ZnO/1%C60-PEG, (c) ZnO/3%C60-PEG and (d) ZnO/5%C60-PEG.


(a)
Current density (mA/cm^2)
Voltage (V)
ZnO
ZnO@0.1% C60-PEG
ZnO@0.5% C60-PEG
ZnO@1% C60-PEG
ZnO@5% C60-PEG
3
0
-3
-6
-9
0.0
0.2
0.4
0.6


(b)
IPCE(%)
Wavelength (nm)
ZnO
ZnO@0.1% C60-PEG
ZnO@0.5% C60-PEG
ZnO@1% C60-PEG
ZnO@5% C60-PEG
60
40
20
0
300
400
500
600
700

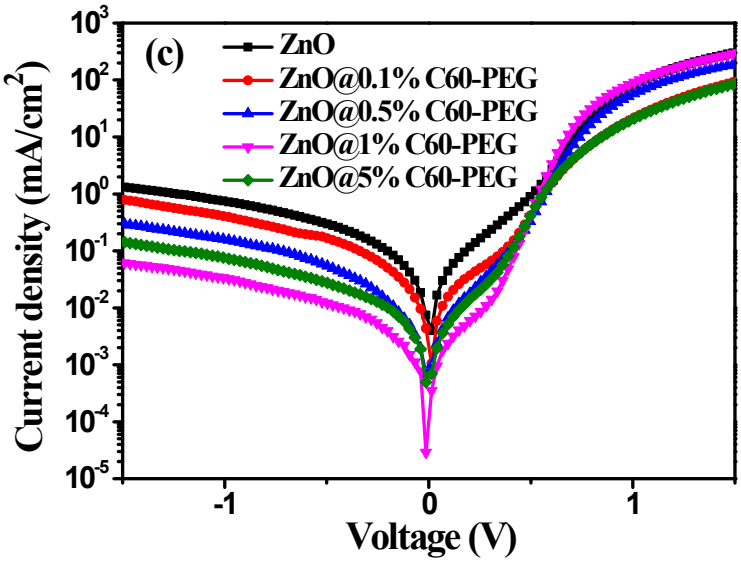
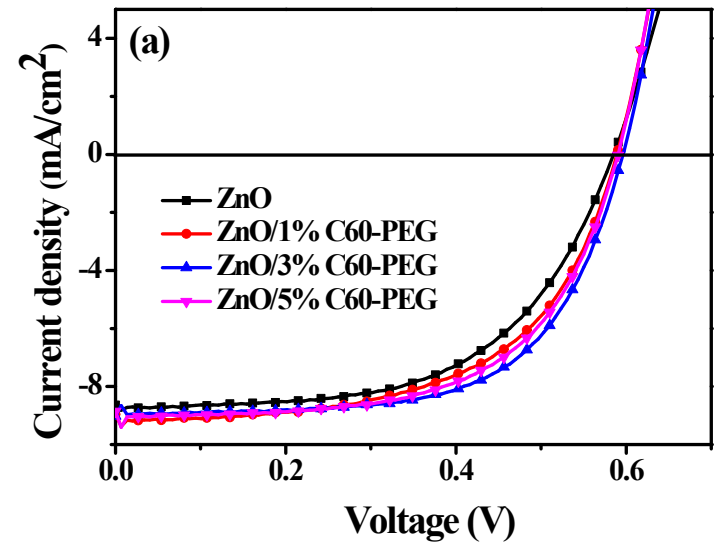
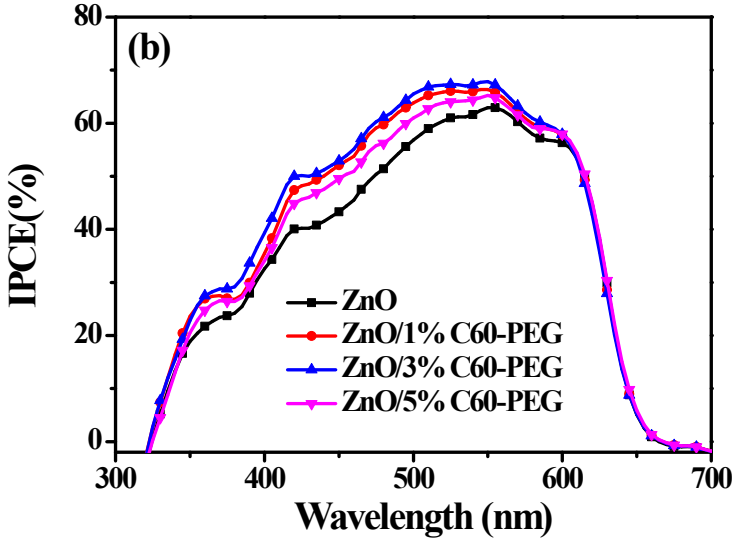


Figure S11. Performance of devices under simulated AM 1.5 G (100 mW·cm^{-2}) illumination. (a) Illuminated *J-V* characteristics, (b) IPCE spectra and (c) *J-V* curve under dark of the devices ITO/cathode buffer layer/P3HT:$PC_{61}BM$/MoO_3/Ag.


(a)
Current density (mA/cm2)
Voltage (V)
ZnO
ZnO/1% C60-PEG
ZnO/3% C60-PEG
ZnO/5% C60-PEG
4
0
-4
-8
0.0
0.2
0.4
0.6


(b)
IPCE(%)
Wavelength (nm)
ZnO
ZnO/1% C60-PEG
ZnO/3% C60-PEG
ZnO/5% C60-PEG
80
60
40
20
0
300
400
500
600
700

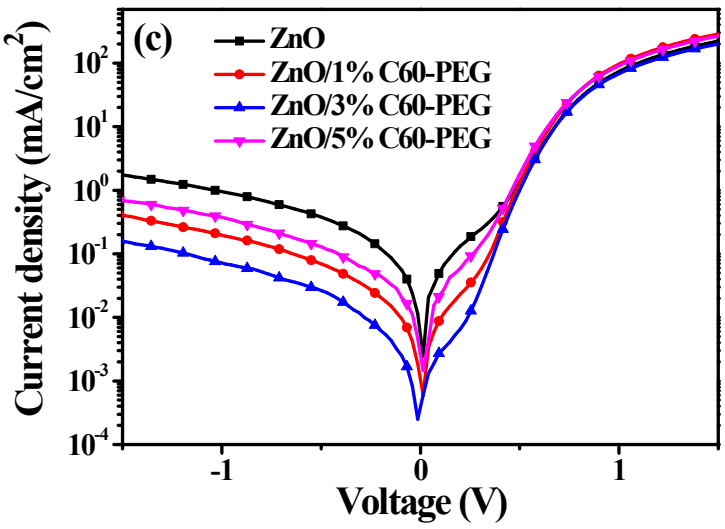


Figure S12. Performance of devices under simulated AM 1.5 G (100 mW·cm^{-2}) illumination. (a) Illuminated *J-V* characteristics, (b) IPCE spectra and (c) *J-V* curve under dark of the devices ITO/cathode buffer layer/P3HT:$PC_{61}BM$/MoO_3/Ag.

Table S4. Photovoltaic parameters of the devices with ITO/cathode buffer layer/P3HT:$PC_{61}BM$/MoO_3/Ag structure. [a]All data of devices had been tested from more than five substrates (20 chips) to ensure reproducibility. [b]The ZnO was synthesized following the process reported by Heeger *et al*. [c]The ZnO was synthesized following the process reported by Beek *et al*.

Device[a]	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF [%]	PCE [%]
ZnO[b]	8.86±0.14	0.599±0.008	57.0±2.1	3.0±0.2
ZnO@0.1%C60-PEG	8.93±0.12	0.623±0.006	60.0±1.6	3.3±0.2
ZnO@0.5%C60-PEG	9.00±0.10	0.622±0.004	62.0±1.3	3.5±0.1
ZnO@1%C60-PEG	**9.29±0.11**	**0.623±0.005**	**64.3±1.1**	**3.7±0.1**
ZnO@5%C60-PEG	8.91±0.13	0.624±0.006	61.8±1.5	3.4±0.2
ZnO[c]	8.64±0.13	0.584±0.007	57.8±1.4	2.9±0.1
ZnO/1%C60-PEG	8.96±0.14	0.588±0.004	58.7±1.7	3.1±0.2
ZnO/3%C60-PEG	**9.02±0.12**	**0.595±0.006**	**62.5±1.2**	**3.4±0.1**
ZnO/5%C60-PEG	8.86±0.12	0.589±0.003	61.4±1.6	3.2±0.1

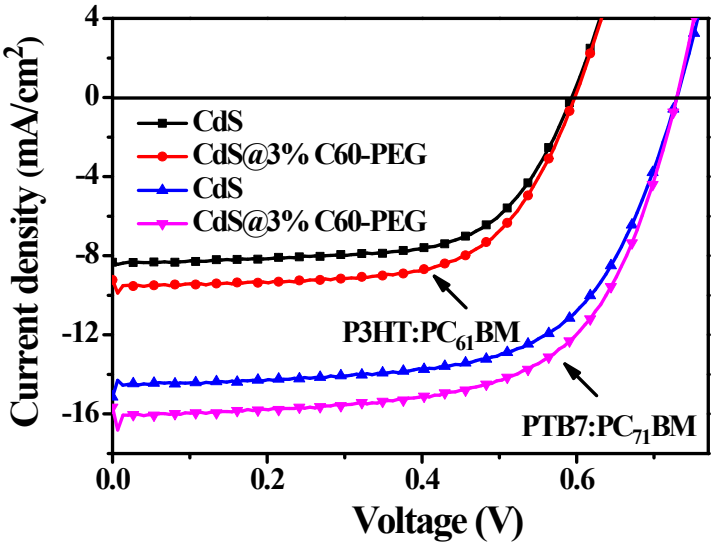


Figure S13. Illuminated *J-V* curves of the devices with ITO/cathode buffer layer/active layer/MoO_3/Ag structure by using CdS and CdS@3%C60-PEG as cathode buffer layer.

Table S5. Photovoltaic parameters of the devices with ITO/cathode buffer layer/active layer/MoO_3/Ag structure. [a]All data of devices had been tested from more than five substrates (20 chips) to ensure reproducibility.

Device[a]	Active Layer	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF [%]	PCE [%]
CdS	P3HT:PC_{61}BM	8.33±0.23	0.593±0.05	64.8±1.2	3.2±0.2
CdS@3% C60-PEG	P3HT:PC_{61}BM	9.22±0.20	0.597±0.04	66.2±1.4	3.6±0.1
CdS	PTB7:PC_{71}BM	15.14±0.12	0.728±0.2	60.9±1.3	6.7±0.1
CdS@3% C60-PEG	PTB7:PC_{71}BM	15.66±0.17	0.728±0.4	64.9±1.5	7.4±0.1

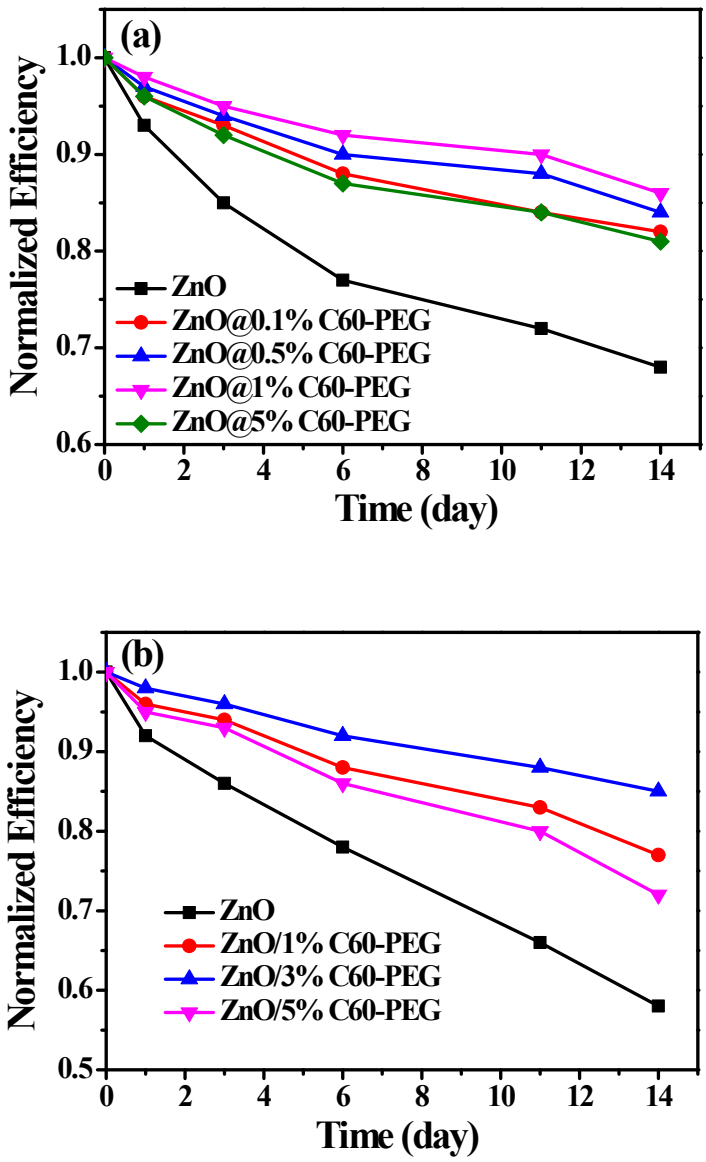


Figure S14. (a) Normalized efficiency decay of inverted devices with ZnO, ZnO@0.1%C60-PEG, ZnO@0.5%C60-PEG, ZnO@1%C60-PEG and ZnO@5%C60-PEG as cathode buffer layer. (b) Normalized efficiency decay of inverted devices with ZnO, ZnO/1%C60-PEG, ZnO/3%C60-PEG and ZnO/5%C60-PEG as cathode buffer layer.