Supplementary Information

Interface engineering through electron transport layer modification for high efficiency organic solar cells

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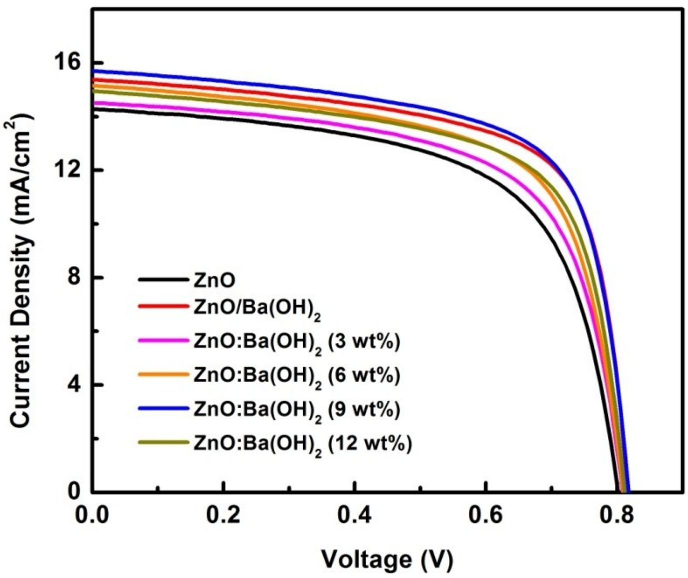

Figure S1 *J-V* characteristics curves under illumination (AM 1.5G, one sun) of devices with ZnO, ZnO/$Ba(OH)_2$ and ZnO:$Ba(OH)_2$ nanocomposite as an ETLs.

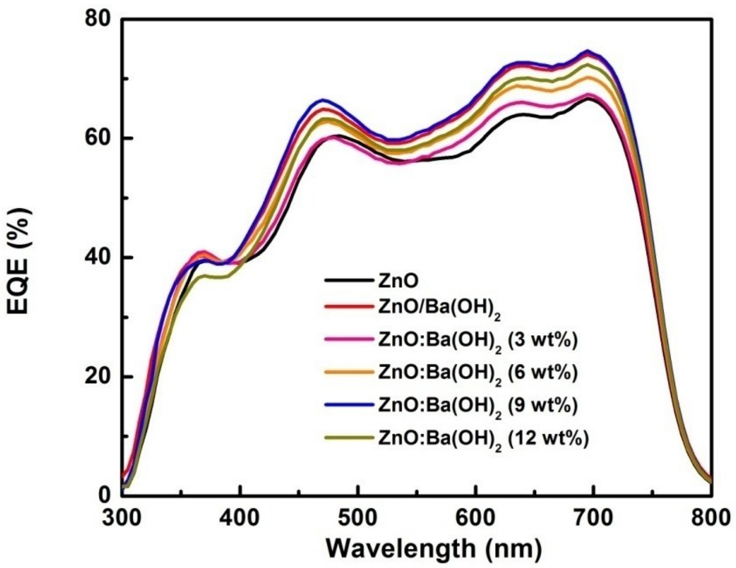

Figure S2 EQE spectra of devices with ZnO, $ZnO/Ba(OH)_2$ and $ZnO:Ba(OH)_2$ nanocomposite as an ETLs.

Table S1 Performance parameters for devices with ZnO, $ZnO/Ba(OH)_2$ and $ZnO:Ba(OH)_2$ nanocomposite as an ETLs.

Electron Transport Layer (ETL)	V_{oc} (mV)	J_{sc}[a] (mA/cm^2)	FF (%)	PCE[b] (%)
ZnO	803	14.28 (14.05)	62.30	7.12 (7.07)
$ZnO/Ba(OH)_2$	814	15.34 (15.56)	68.20	8.54 (8.46)
$ZnO:Ba(OH)_2$ (3wt%)	803	14.50 (14.33)	63.90	7.44 (7.39)
$ZnO:Ba(OH)_2$ (6wt%)	810	15.15 (14.90)	65.10	7.98 (7.92)
$ZnO:Ba(OH)_2$ (9wt%)	818	15.69 (15.70)	67.60	8.66 (8.59)
$ZnO:Ba(OH)_2$ (12wt%)	813	14.95 (15.07)	66.60	8.07 (8.01)

[a] Jsc as calculated from EQE is shown in parentheses. [b] The average PCE is shown in parentheses. Average PCE was calculated using the results of 5 devices.

Table S1a Comparison of performance parameters for PTB7-Th: PCBM devices with ZnO, $ZnO/Ba(OH)_2$ and $ZnO:Ba(OH)_2$ nanocomposite as an ETLs with the previously reported similar studies.

Work	Cathode configuration	Anode Configuration	V_{oc} (mV)	J_{sc}[a] (mA/cm^2)	FF (%)	PCE[b] (%)
Present	ITO/ $ZnO/Ba(OH)_2$	MoO_3/Ag	814	15.34 (15.56)	68.20	8.54 (8.46)
Present	ITO/ $ZnO:Ba(OH)_2$ (9wt%)	MoO_3/Ag	818	15.69 (15.70)	67.60	8.66 (8.59)
Previous[1]	ITO/patterned ZnO	MoO_3/Al	780	19.47	66.90	10.10
Previous[2]	ITO/IZO	MoO_3/Ag	790	16.42	70.2	9.11
Previous[3]	ITO/AZO	MoO_3/Ag	800	17.70	70.70	9.94
Previous[4]	ITO/PFN	MoO_3/Al	830	17.43	73.80	10.61
Previous[5]	ITO/C 60 –SB	MoO_3/Ag	750	18.24	66.00	9.08
Previous[6]	ITO/ZnO:PBI-H	MoO_3/Al	820	17.69	72.90	10.59
Previous[7]	ITO/ZnO/[BMIM] BF 4	MoO_3/Ag	780	17.70	73.50	10.15
Previous[8]	ITO/ZnO–C 60	MoO_3/Ag	800	15.73	74.30	9.35

[a] Jsc as calculated from EQE is shown in parentheses. [b] The average PCE is shown in parentheses. Average PCE was calculated using the results of 5 devices.

Table S1b Conductivities of ZnO, ZnO/$Ba(OH)_2$ and ZnO:$Ba(OH)_2$ nanocomposite thin films

Electron Transport Layer (ETL)	Conductivity (S/cm)
ZnO	51.9×10^{-3}
ZnO/$Ba(OH)_2$	91.4×10^{-3}
ZnO:$Ba(OH)_2$ (3wt%)	74.8×10^{-3}
ZnO:$Ba(OH)_2$ (6wt%)	75.2×10^{-3}
ZnO:$Ba(OH)_2$ (9wt%)	93.2×10^{-3}
ZnO:$Ba(OH)_2$ (12wt%)	89.3×10^{-3}

Table S2 Contact angle of the surface of films of ZnO, ZnO/$Ba(OH)_2$ and ZnO:$Ba(OH)_2$ nanocomposite thin films deposited on ITO coated glass substrates.

Electron Transport Layer (ETL)	Contact Angle (in deg)
ZnO	46.88 ± 0.65
ZnO/$Ba(OH)_2$	49.59 ± 0.54
ZnO:$Ba(OH)_2$ (3wt%)	47.98± 0.60
ZnO:$Ba(OH)_2$ (6wt%)	52.09 ± 1.59
ZnO:$Ba(OH)_2$ (9wt%)	52.65 ± 0.81
ZnO:$Ba(OH)_2$ (12wt%)	51.75 ± 0.87

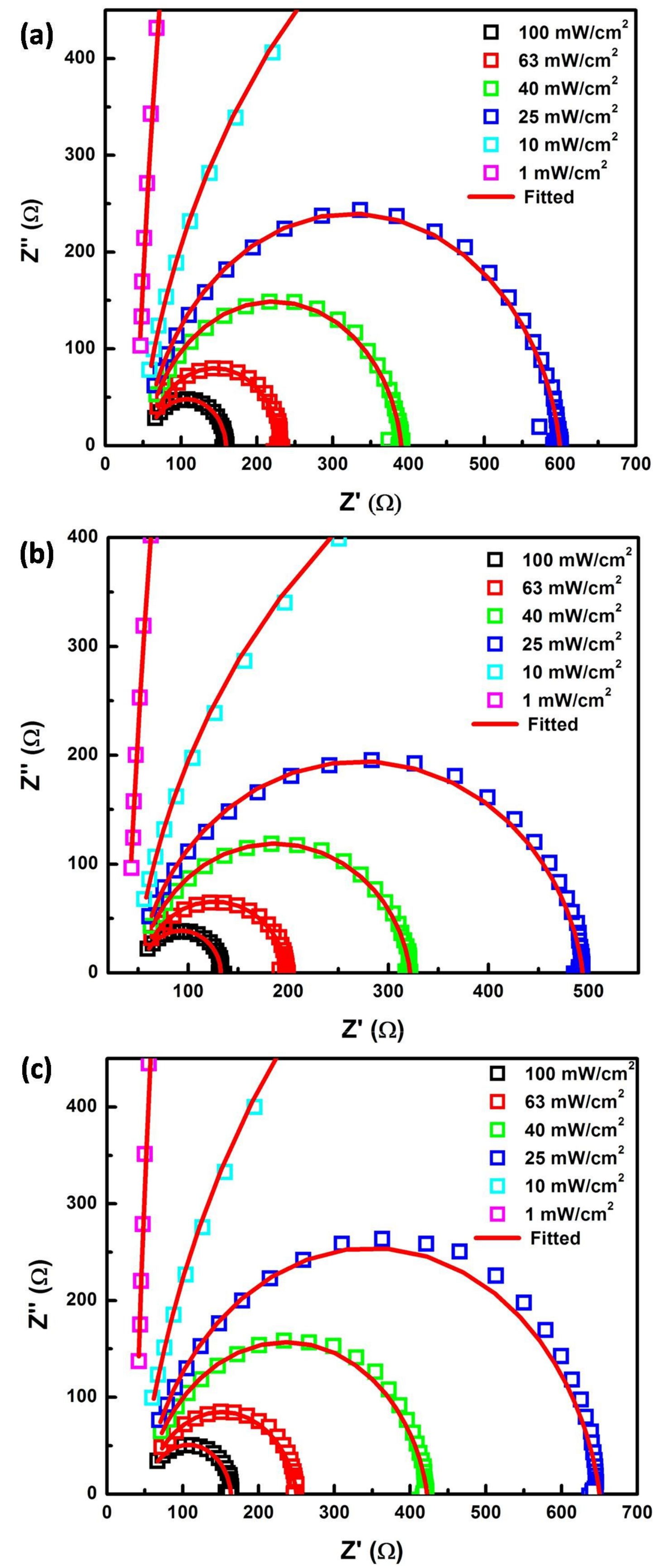

Figure S3 Nyquist plots of PTB7-Th:$PC_{70}BM$ OSCs with (a) ZnO (b) ZnO/$Ba(OH)_2$ and (c) ZnO:$Ba(OH)_2$ nanocomposite as an ETLs under different white light illumination intensities

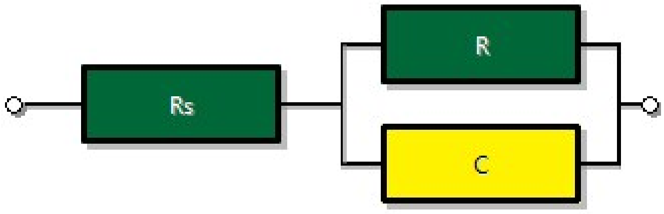

Figure S4 Equivalent circuit used for fitting for different impedance curves.

Table S3 Order of recombination for devices with ZnO, ZnO/$Ba(OH)_2$ and ZnO:$Ba(OH)_2$ nanocomposite as an ETLs.

Electron Transport Layer (ETL)	α	β	λ (from Fig 6 (c))	λ (from Eq (7))
ZnO	0.29	0.70	3.93	1.36
ZnO/$Ba(OH)_2$	0.27	0.86	2.75	2.12
ZnO:$Ba(OH)_2$ (9 wt%)	0.25	0.76	2.32	2.03

References:

1 J. De Chen, C. Cui, Y. Q. Li, L. Zhou, Q. D. Ou, C. Li, Y. Li and J. X. Tang, *Adv. Mater.*, 2015, 27, 1035–1041.

2 S. H. Liao, H. J. Jhuo, P. N. Yeh, Y. S. Cheng, Y. L. Li, Y. H. Lee, S. Sharma and S. A. Chen, *Sci. Rep.*, 2014, 4, 4–10.

3 L. K. Jagadamma, M. Al-Senani, A. El-Labban, I. Gereige, G. O. Ngongang Ndjawa, J. C. D. Faria, T. Kim, K. Zhao, F. Cruciani, D. H. Anjum, M. A. McLachlan, P. M. Beaujuge and A. Amassian, *Adv. Energy Mater.*, 2015, 5, 1–12.

4 Z. He, B. Xiao, F. Liu, H. Wu, Y. Yang, S. Xiao, C. Wang, T. P. Russell and Y. Cao, *Nat. Photonics*, 2015, 9, 174–179.

5 Y. Liu, Z. Page, S. Ferdous, F. Liu, P. Kim, T. Emrick and T. Russell, *Adv. Energy Mater.*, 2015, 5, 1–6.

6 L. Nian, W. Zhang, N. Zhu, L. Liu, Z. Xie, H. Wu, F. Würthner and Y. Ma, *J. Am. Chem. Soc.*, 2015, 137, 6995–6998.

7 W. Yu, L. Huang, D. Yang, P. Fu, L. Zhou, J. Zhang and C. Li, *J. Mater. Chem. A*, 2015, 3, 10660–10665.

8 S. H. Liao, H. J. Jhuo, Y. S. Cheng and S. A. Chen, *Adv. Mater.*, 2013, 25, 4766–4771.