

Supporting Information

Reduction of Charge Recombination in PbS Colloidal Quantum Dot Solar Cells at the Quantum Dot/ZnO Interface by Inserting a MgZnO Buffer Layer

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Table S1. Details of SCAPS simulation used parameters.

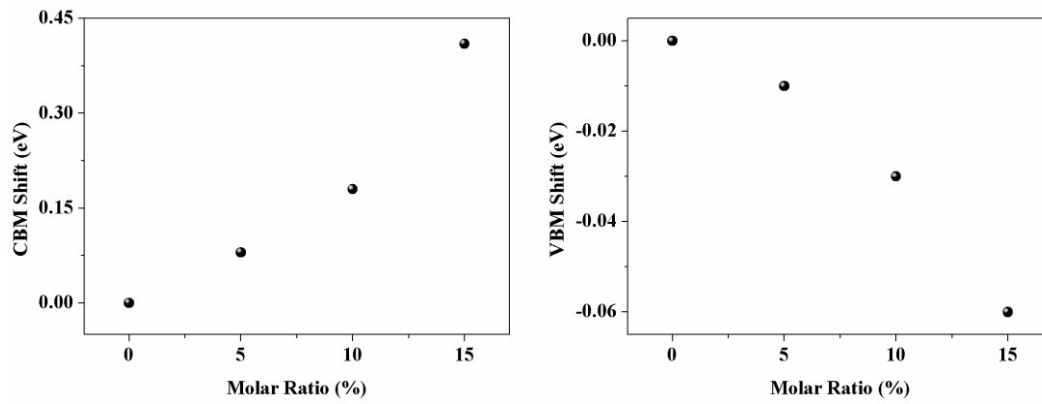


Figure S1. CBM and VBM as function of molar ratio of Mg in MZO film. Values obtained from reference.¹

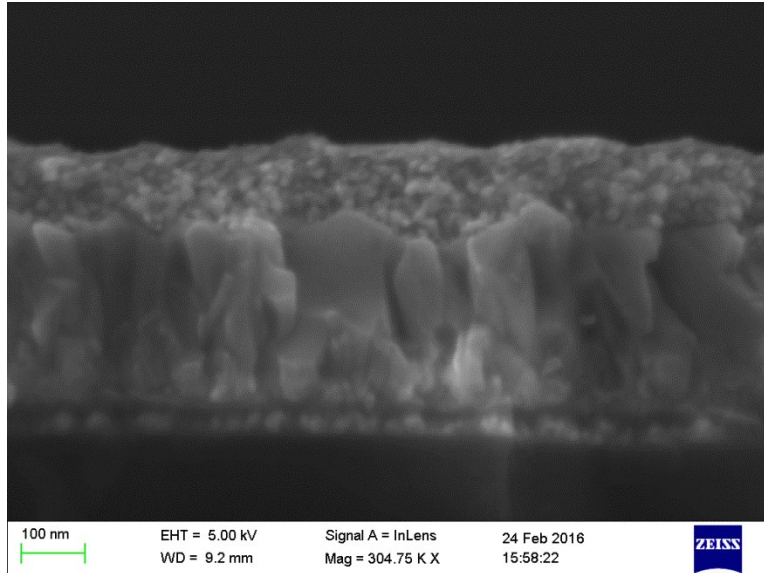


Figure S2. Cross-sectional SEM image of ZnO/MZO electrode covered FTO glass.

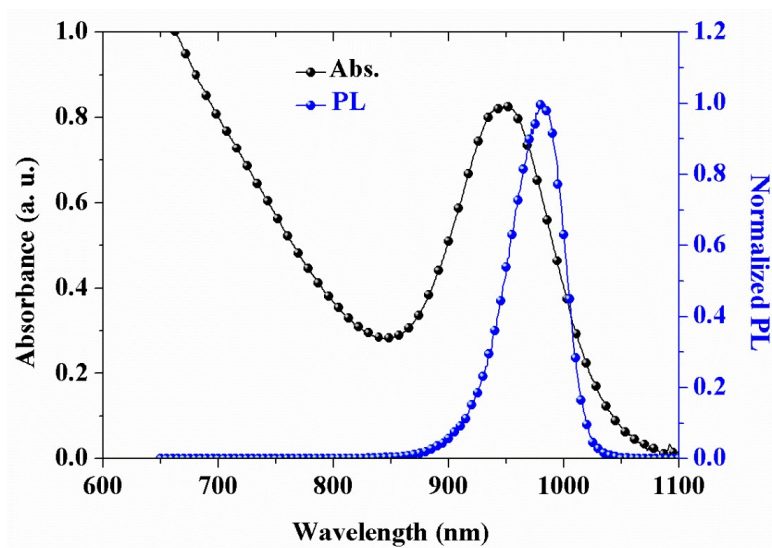


Figure S3. Light absorption and normalized photoluminescence spectra of PbS CQDs in octane.

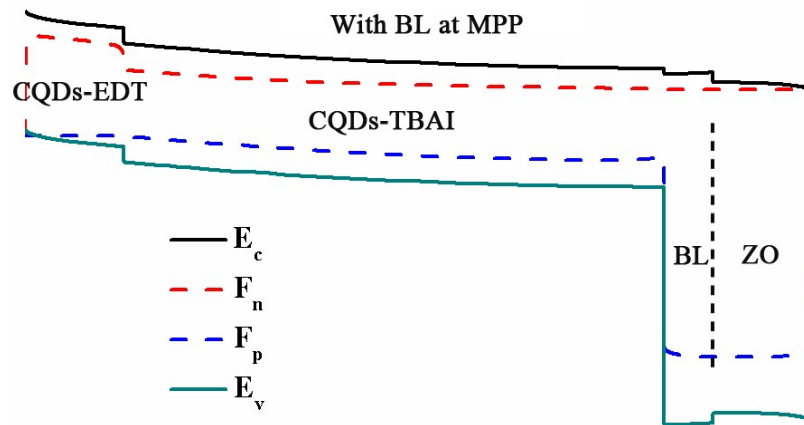


Figure S4. Band diagram within the CQD solar cell with a BL at maximum power point. The CBM up-shift 0.1 eV referring to ZnO layer

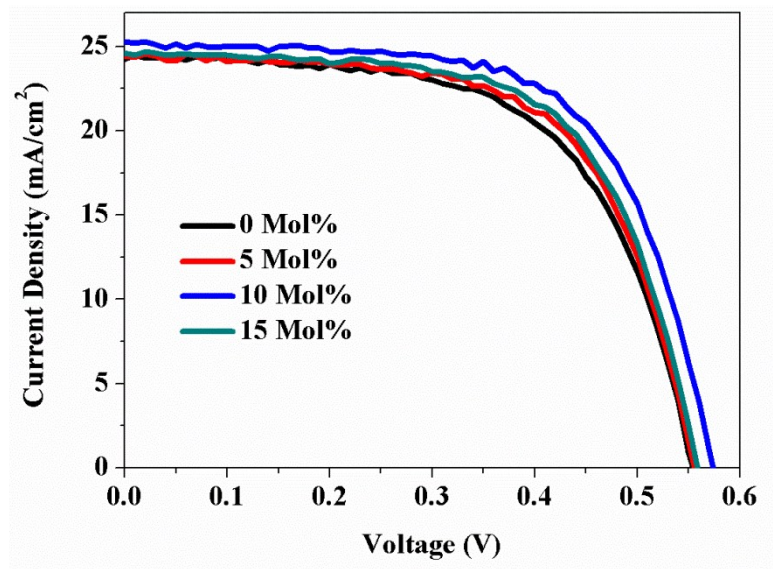


Figure S5. J - V curves of the solar cells with a MZO-BL as a function of molar ratio of magnesium in MZO layer.

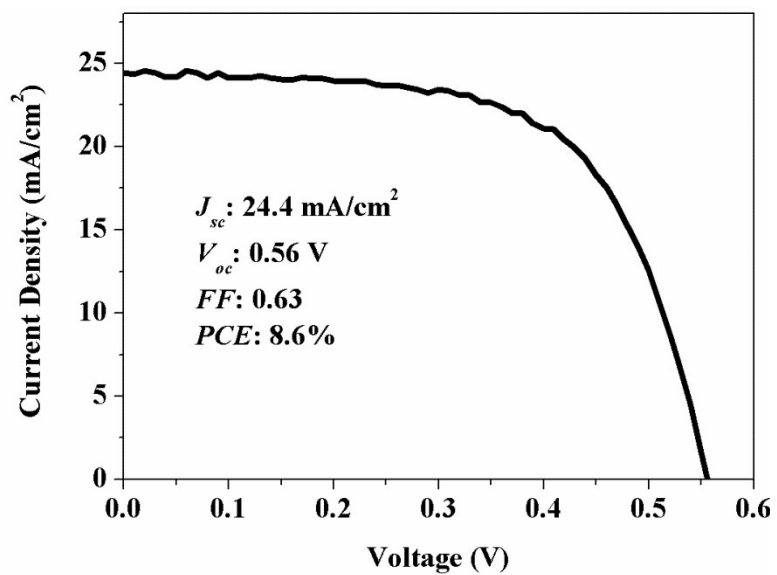


Figure S6. *J-V* curve of the solar cell with a MZO film as electron collecting layer.

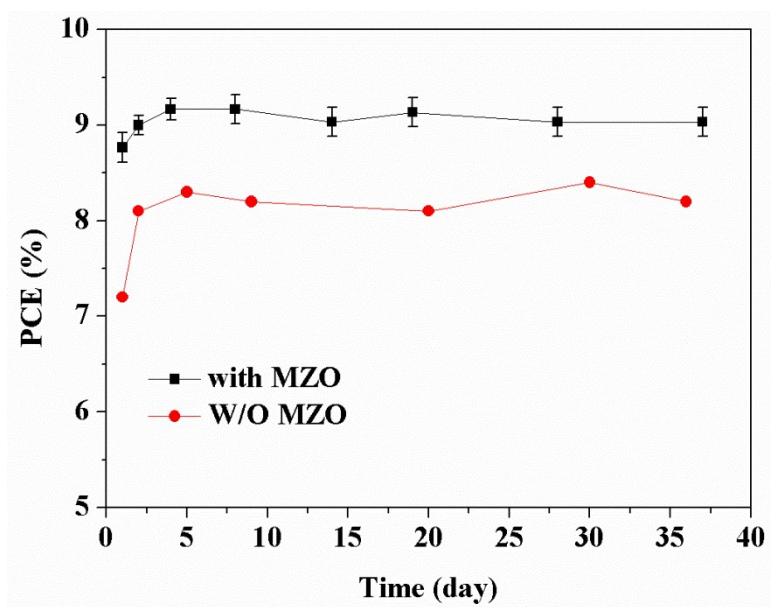


Figure S7. The stability test of CQD solar cell with a MZO-BL and without any BLs (ZnO only). The unsealed solar cells were stored in ambient atmosphere under dark condition.

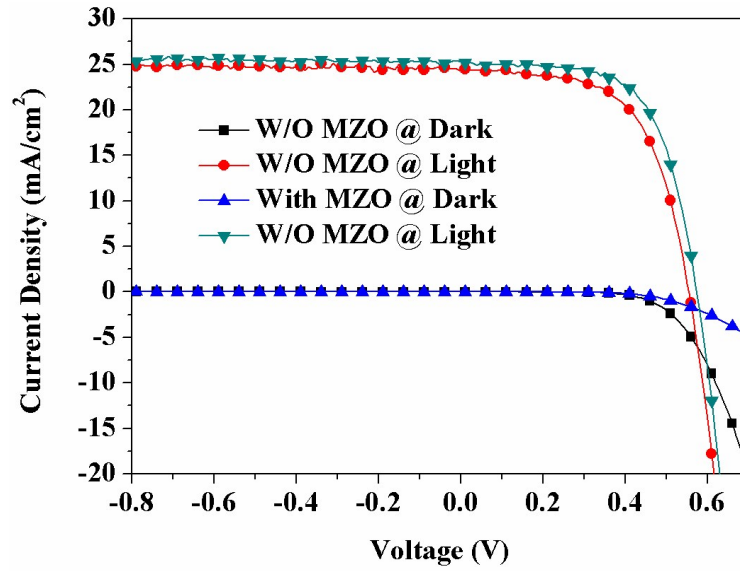


Figure S8. J - V curves of the solar cell without any BLs and with a MZO-BL under dark and illumination condition.

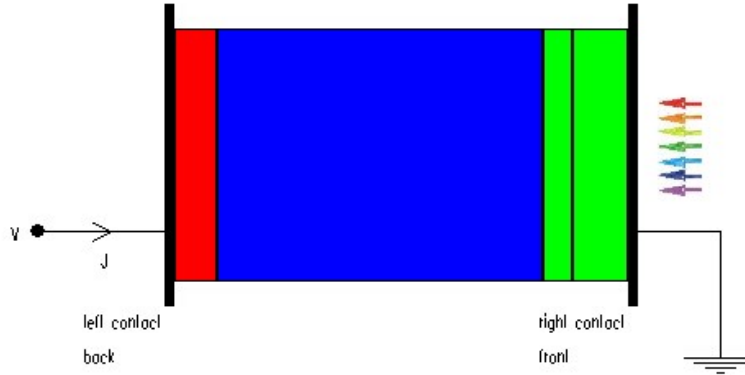


Figure S9. Model figure from SCAPS simulation.

Table S1. Details of SCAPS simulation used parameters. Part of these parameters are taken from literatures.^{2,3}

	PbS-TBAI	PbS-EDT	ZnO(or MZO)
Thickness (nm)	230	50	60 (40+20)
Bandgap edge (eV)	1.2	1.2	3.2(or up shift)
Electron affinity (eV)	4.15	3.9	4.3
Permittivity (ϵ_r)	20	20	66
CB/VB DOS (cm^{-3})	1E19	1E19	1E19
Electron mobility (cm^2/Vs)	2E-2	2E-4	5E-2
Ndonor (cm^{-3})	1E15	1E14	1E17
Nacceptor (cm^{-3})	1E15	1E16	0
EDT/TBAI defect (neutral)	total density (integrated over all energies) ($1/\text{cm}^2$): 1.00E+16		
Capture cross section (cm^2)	1.2E-13	1.2E-13	
Position below E_c (eV)	0.5	0.5	
Density (cm^{-3})	1E16	1E16	
TBAI-ZnO interface defects (neutral)	total density (integrated over all energies) ($1/\text{cm}^2$): 1.00E+16		
Capture cross section (cm^2)			1E-19
Position above E_v (eV)			0.6
Density (cm^{-3})			1E16

References

1. L. Hu, D. B. Li, L. Gao, H. Tan, C. Chen, K. H. Li, M. Li, J. B. Han, H. S. Song, H. Liu, and J. Tang, *Adv. Funct. Mater.* **2016**, *26*, 1899-1907.
2. G. H. Kim, F. P. Garcia de Arquer, Y. J. Yoon, X. Lan, M. Liu, O. Voznyy, Z. Yang, F. Fan, A. H. Ip, P. Kanjanaboos, S. Hoogland, J. Y. Kim, and E. H. Sargent, *Nano Lett.* **2015**, *15*, 7691-7696.
3. M. Liu, F. P. de Arquer, Y. Li, X. Lan, G. H. Kim, O. Voznyy, L. K. Jagadamma, A. S. Abbas, S. Hoogland, Z. Lu, J. Y. Kim, A. Amassian, and E. H. Sargent, *Adv. Mater.* **2016**, *28*, 4142-4148.