Electronic Supplementary Material (ESI) for Nanoscale.

Low-temperature Solution-Processed Indium Incorporated Zinc Oxide Electron Transport Layer for High-efficiency Lead Sulfide Colloidal Quantum Dot Solar Cells

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Table. S1. $E_{on\text{-}set}$, $E_{cut\text{-}off}$ and VBM values of ZnO, IZO, AZO, and GZO films.

ETLs	$E_{on\text{-}set}$ (eV)	$E_{cut\text{-}off}$ (eV)	VBM (eV)
ZnO	3.57	17.1	7.67
IZO	3.54	16.78	7.96
AZO	3.51	17.0	7.71
GZO	3.45	16.9	7.75

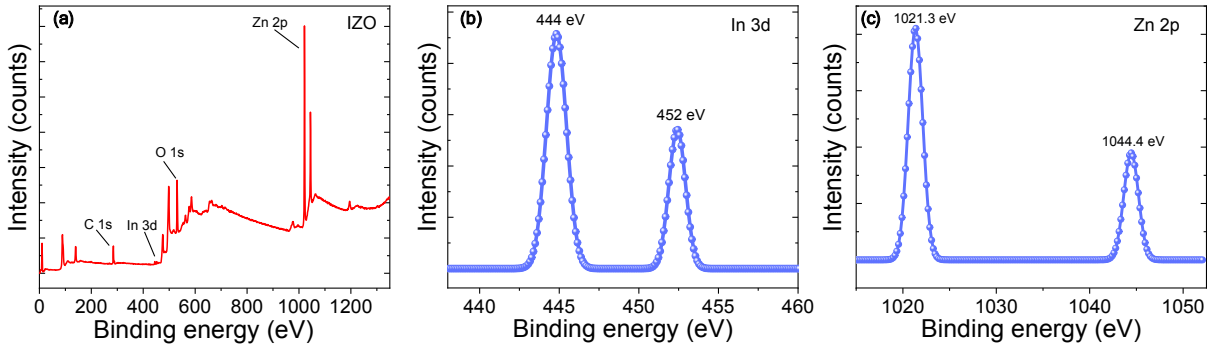

Fig. S1. XPS spectra of the IZO film. (a) Broad scan survey. (b-d) XPS spectra of In 3d, and Zn 2p, respectively. The XPS spectra of the In 3d and Zn 2p are quite symmetric, indicative of the only one valence state, i.e. In^{3+} and Zn^{2+} based on the evaluation on the binding energies of In 3d (444 and 452 eV) and Zn 2p (1021.3 and 1044.4 eV).[1, 2] The binding energy and FWHM values for Zn 2p, In 3d, and O1s are also given in Table S1.

Table S2. Peak position and FWHM of the XPS for the IZO.

Levels	Peaks (eV)	FWHM
In 3d	444.0	1.48
	451.4	1.23
Zn 2p	1021.3	1.83
	1044.4	1.86
O 1s	529.3	1.14
	531.2	2.44

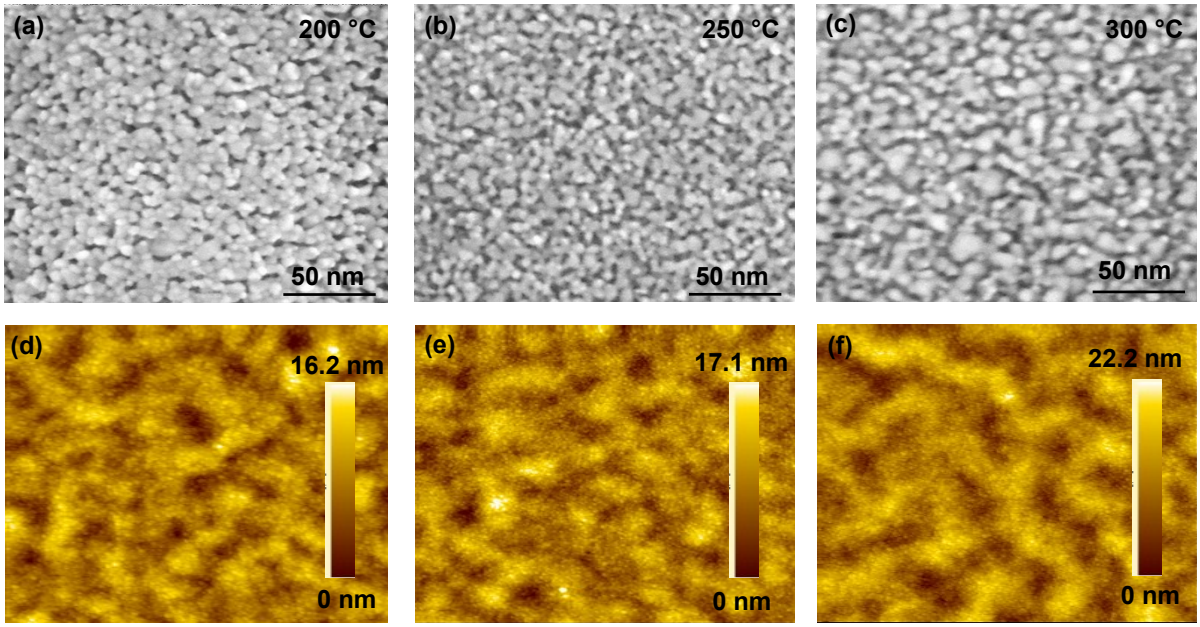

Fig. S2. SEM and AFM images of the IZO films annealed at 200 ℃, 250 ℃, 300 ℃, respectively. The particle sizes are slightly increased with increasing the annealing temperatures from the SEM observations, which are consistent with the AFM characterizations that reveal similarly the gradually increased surface roughness.

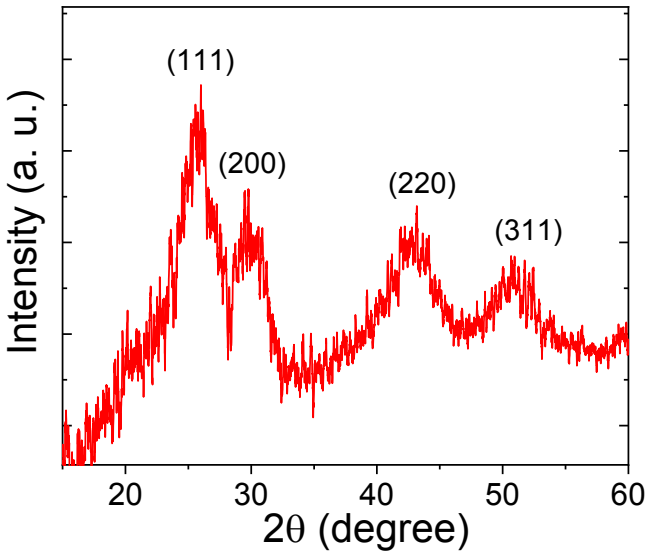

Fig. S3. XRD pattern of PbS CQDS.

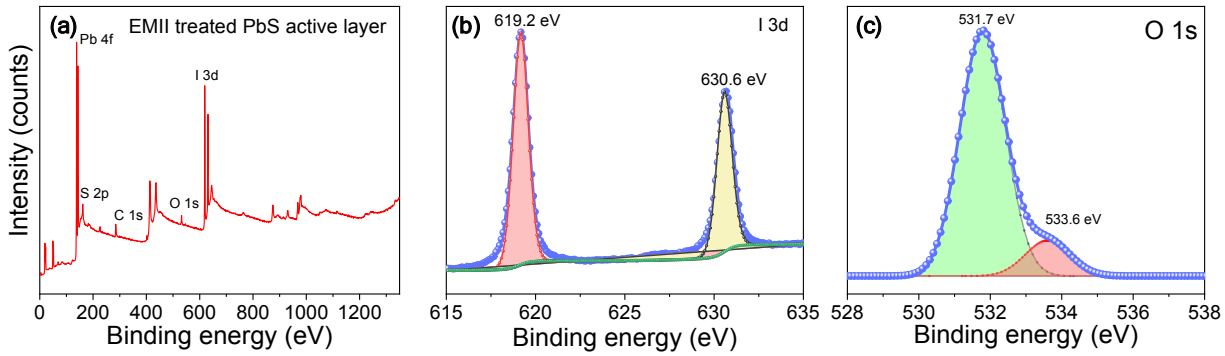

Fig. S4. XPS spectra of the PbS-EMII film. (a) Broad scan survey. (b) XPS peaks of I 3d. (c) XPS peaks of O 1s. The broad scan spectrum gives all the XPS components. It is well known that the O 1s spectrum can describe different organics groups that contain oxygen (like COO- and -OH groups) linked to (111) facets of PbS CQDs, which are regarded as the primary source of trap states.[3-5] The peaks of O 1s can be deconvoluted into two species, which derive from a functional group of Pb-OH (531.7 eV) and COO-Pb (533.6 eV).

Table S3. Peak position and FWHM of the XPS for the PbS-EMII.

PbS-EMII	Peaks (eV)	FWHM
Pb 4f	138.12	0.90
	142.9	0.91
I 3d	619.2	1.14
	630.6	0.47
S 2p	161.1	0.88
	162.3	0.67
O 1s	531.7	1.49
	533.6	1.47

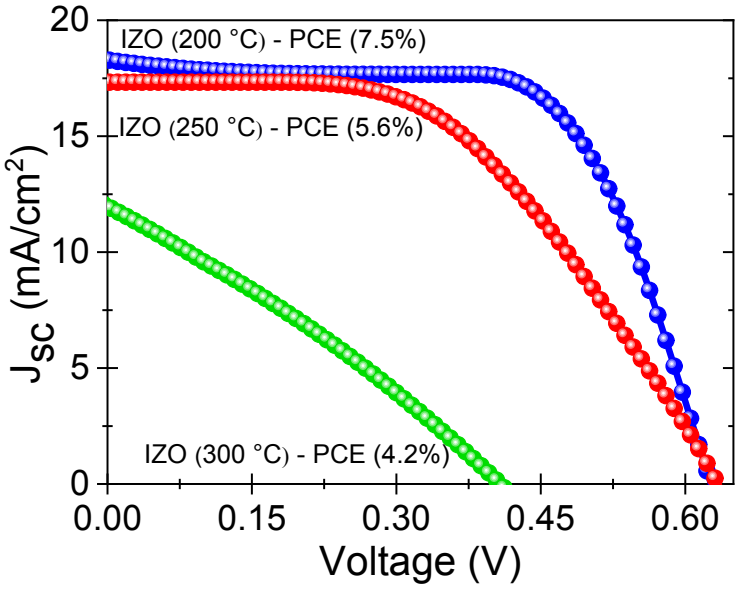

Fig. S5. J-V curves of IZO based PbS CQDSCs annealed at 200 ℃, 250 ℃, 300 ℃, respectively. It is clear that the solar cell devices demonstrate a worse PCE with the increased annealing temperatures, e.g. the PCE decreases from 7.5% (200 ℃) to 4.2% (300 ℃). Similarly, the FF also decreases from 66% (200 ℃) to only 32% (300 ℃), which could be associated with the increase in series resistance (R_S) as well as the shunt resistance (R_{Sh}).[6]

Table S4. Summarized solar cell parameters for ZnO and IZO based on 60 devices.

Device		PCE (%)	FF (%)	*Voc* (V)	*Jsc* ($mAcm^{-2}$)
ZnO/PbS	Best	9.4	63	0.61	24.3
	Average	9.13 ± 0.26	62.87 ± 0.4	0.60 ± 0.01	23.98 ± 0.85
IZO/PbS	Best	11.1	68	0.64	25.8
	Average	10.96 ± 0.19	67.50 ± 0.5	0.63 ± 0.009	25.71 ± 0.09

References

1. H. J. Kim, K. W. Seo, Y. J. Noh, S. I. Na, A. Sohn, D. W. Kim and H. K. Kim, *Sol. Energy Mater. Sol. Cells*, 2015, **141**, 194-202.
2. L. Wang, F. Liu, X. Cai, T. Ma and C. Jiang, *J. Phys. Chem. C*, 2018, **122**, 28491-28496.
3. M. Yuan, M. Liu and E. H. Sargent, *Nat. Energy*, 2016, **1**, 1-9.
4. Y. Cao, A. Stavrinadis, T. Lasanta, D. So and G. Konstantatos, *Nat. Energy*, 2016, **1**, 1-6.
5. D. Zherebetskyy, M. Scheele, Y. Zhang, N. Bronstein, C. Thompson, D. Britt, M. Salmeron, P. Alivisatos and L. W. Wang, *Science*, 2014, **344**, 1380-1384.
6. I. Jeon, J. W. Ryan, T. Nakazaki, K. S. Yeo, Y. Negishi and Y. Matsuo, *J. Mater. Chem. A*, 2014, **2**, 18754-18760.