Electronic Supplementary Information

Dimension engineering on cesium lead iodide for efficient and stable perovskite solar cell

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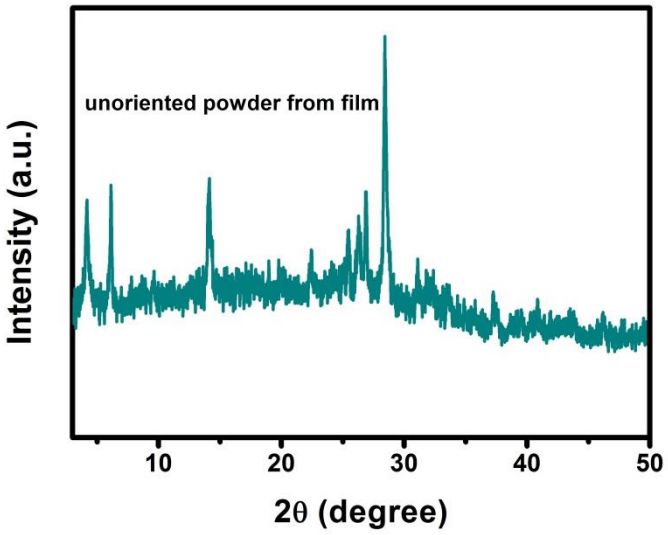

Fig. S1 PXRD patterns of $BA_2CsPb_2I_7$ powder scraped from the film.

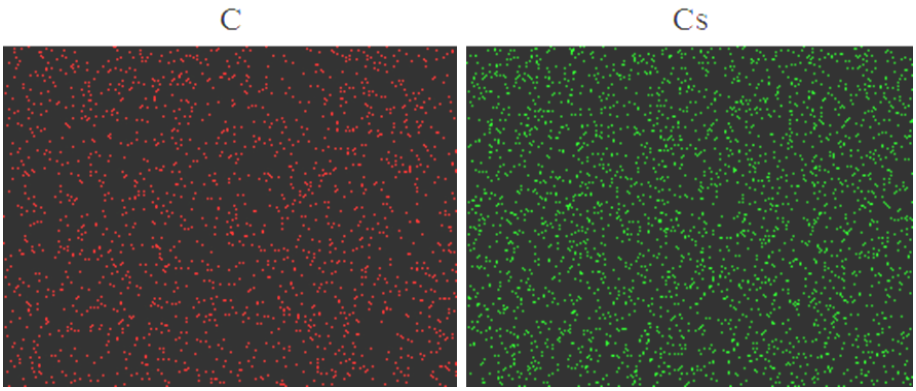

Fig. S2 EDX elemental mapping of C and Cs in $BA_2CsPb_2I_7$ film.

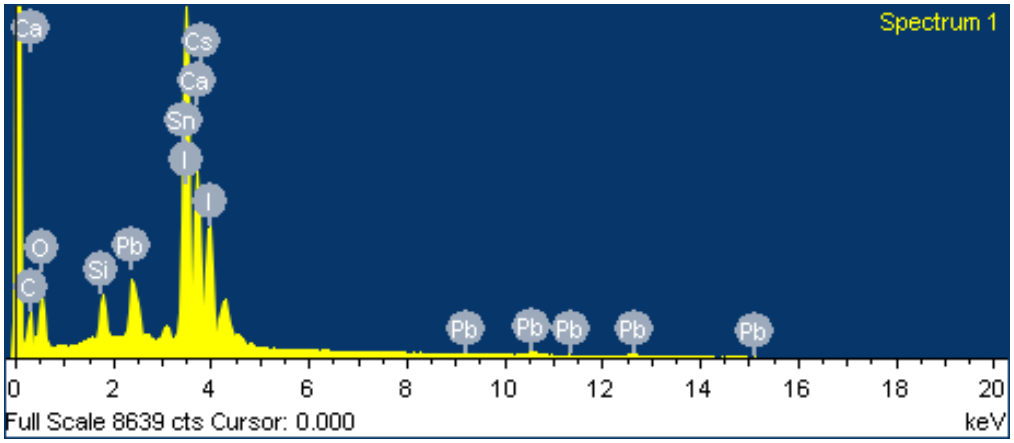

Fig. S3 SEM-EDX elemental analysis of $BA_2CsPb_2I_7$ perovskite film.

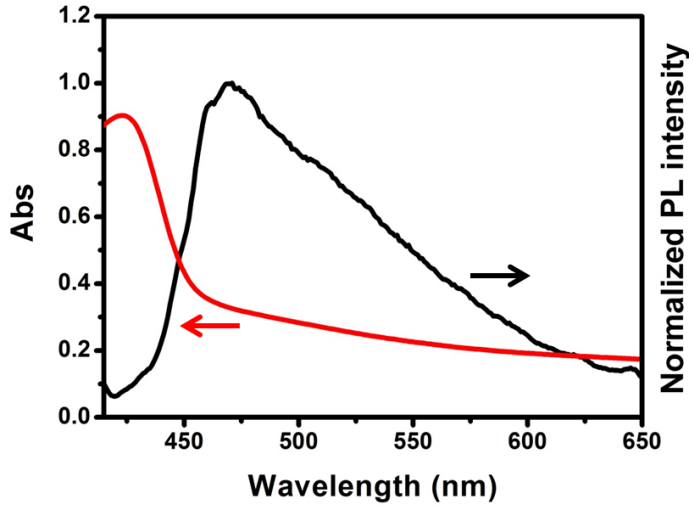

Fig. S4 (a) Absorption spectra and (b) fluorescence spectra of thin films of n-$CsPbI_3$

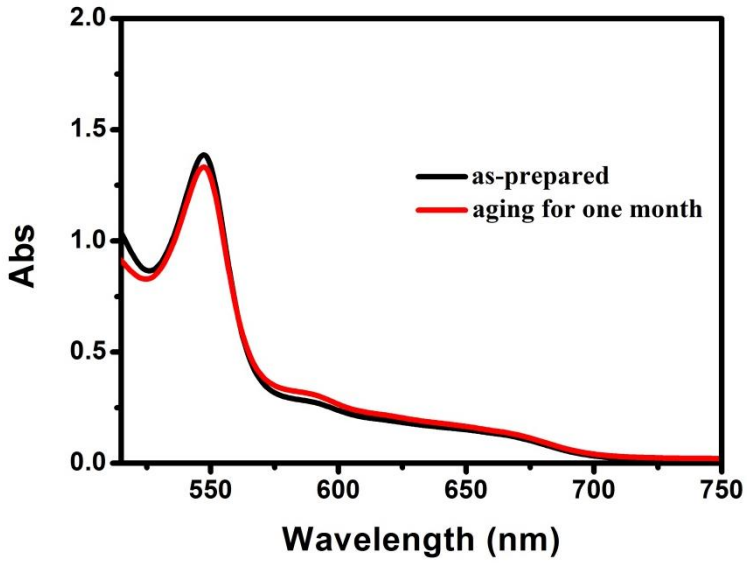

Fig. S5 Absorption spectra of $BA_2CsPb_2I_7$ film before and after exposure to 30% relative humidity for one month.

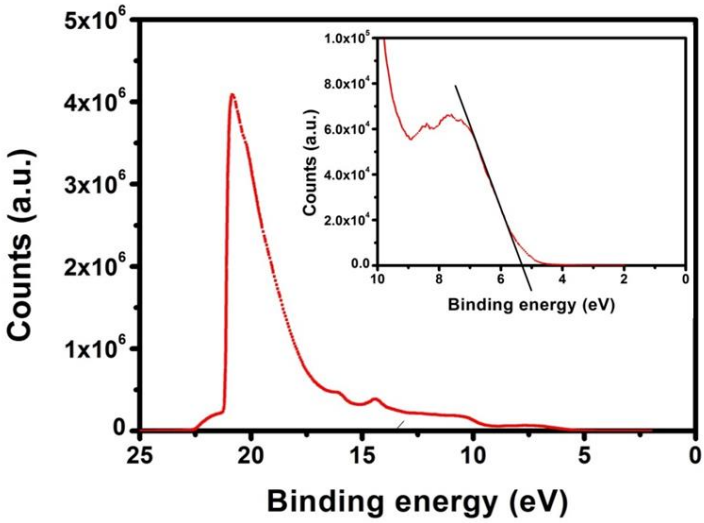

Fig. S6 Ultraviolet photoelectron spectrum (UPS) of the $BA_2CsPb_2I_7$. The binding energy is calibrated with respect to He I photon energy (21.21 eV). The valence band energy can be estimated to be ~5.4 eV below vacuum level.

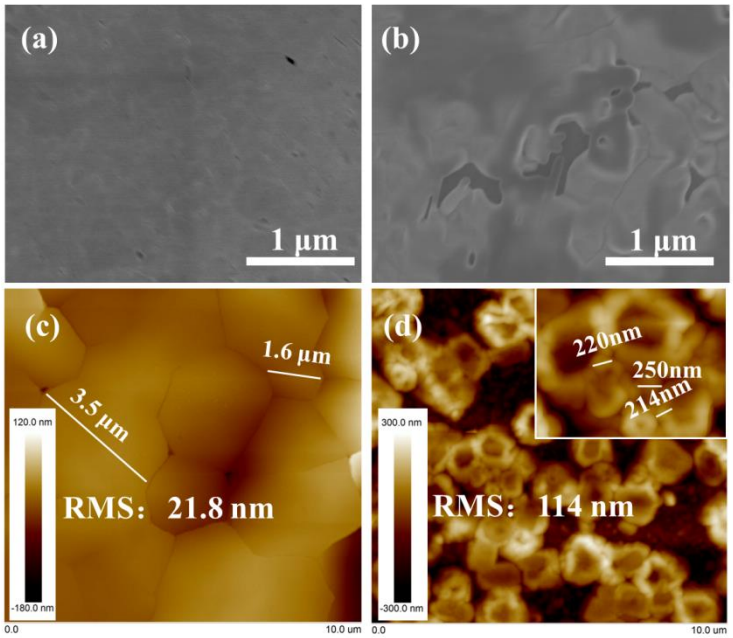

Fig. S7 Top view SEM image of (a) $BA_2CsPb_2I_7$ perovskite film and (b) $CsPbI_3$ film. And AFM topography (c) $BA_2CsPb_2I_7$ perovskite film and (d) $CsPbI_3$ film.

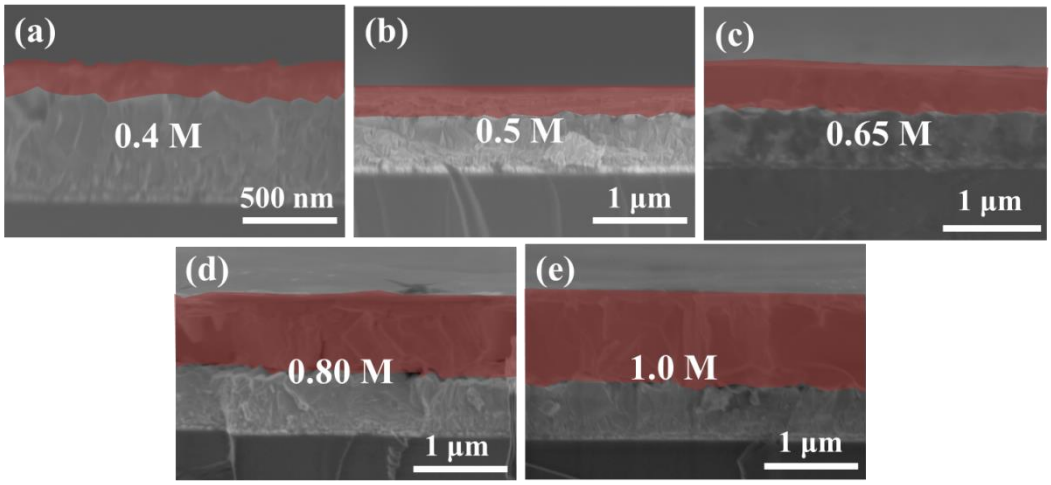

Fig. S8 Cross-sectional SEM images of $BA_2CsPb_2I_7$ films prepared with different precursor concentration.

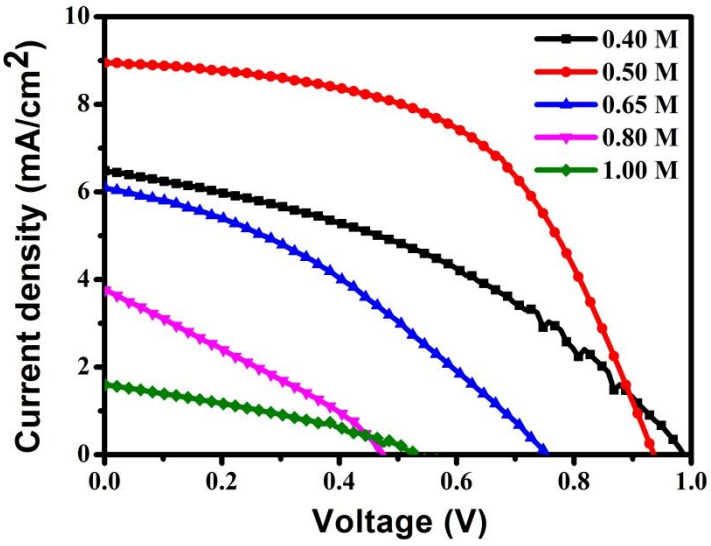

Fig. S9 *J-V* curves of planar $BA_2CsPb_2I_7$-based devices with different precursor concentration.

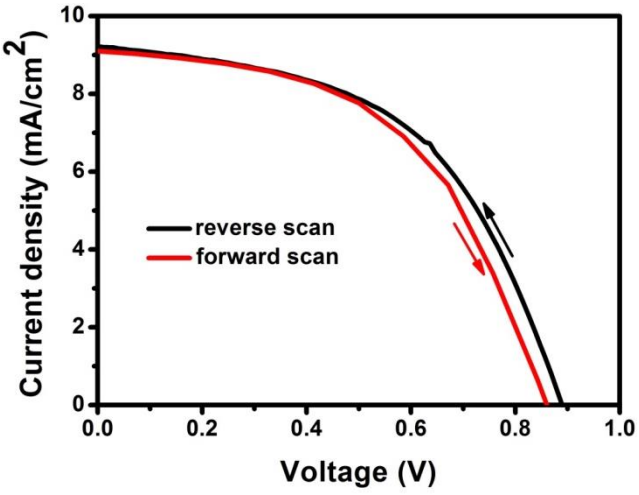

Fig. S10 The *J-V* curves and photovoltaic parameters were performed with reverse scan (forward bias to short circuit) and forward scan (from short circuit to forward bias).

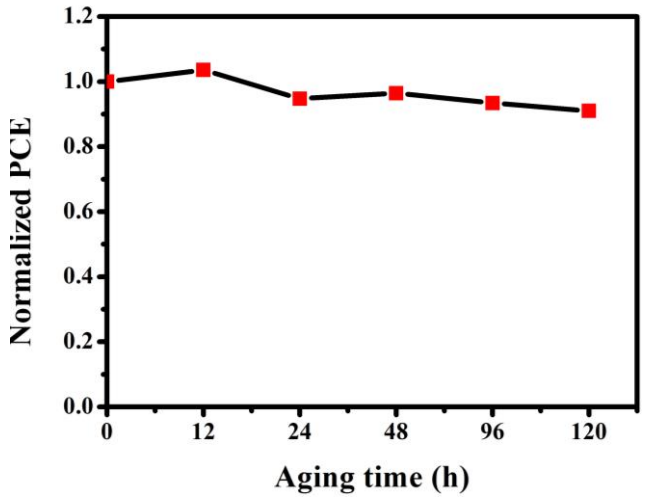

Fig. S11 Photo-stability test under constant light white illumination (0.7 sun) for $BA_2CsPb_2I_7$ perovskite devices without any encapsulation.

Table S1 SEM-EDX elemental analysis of $BA_2CsPb_2I_7$ perovskite film

Element	Weight %	Atomic %
Cs	2.47	0.89
Pb	7.37	1.71
I	16.40	6.23

Experimental Cs:I:Pb ratio: 1:1.92:7. (For the purpose of only comparing Cs:Pb:I ratio, we do not include atomic% elements such as C, O, Si, Ca, Sn.)

Table S2 Photovoltaic performance of $BA_2CsPb_2I_7$-based devices with different precursor concentrations.

Concentration	J_{sc} [mA cm^{-2}]	V_{oc} [mV]	PCE [%]	*FF*
0.4 M	6.49	987	2.557	0.399
0.5 M	8.88	957	4.839	0.570
0.65M	6.10	754	1.625	0.353
0.80 M	3.76	476	0.522	0.291
1.0 M	1.60	530	0.284	0.334

Table S3 Comparison of power conversion efficiency (PCE), perovskite film annealing temperature and long-term stability of $CsPbI_3$-based perovskite solar cells.

Material	Annealing temperature	PCE	Long-term stability	Ref
$BA_2CsPb_2I_7$	100 ^{o}C	4.84%	85 ^{o}C for 3 days; 30% RH for 30 days	This work
$CsPbI_3$	100 ^{o}C	2.9%	Stable for hours in air	1
$CsPbI_3$	100 ^{o}C	4.13%	<30% RH for 72 h	2
$CsPbI_3$	350 ^{o}C	4.61%	Not stable	3
$CsPbI_3$ QDs	180 ^{o}C	10.5%	Stored in desiccator in dark	4

			for 60 days	
$CsPbI_2Br$	250 ^oC	9.7%	85 ^oC for 3h; 50% RH for 1h	5
$CsPbI_2Br$	65^oC and then 135 ^oC	6.69%	180 ^oC for 30 min	6
$CsPbIBr_2$	250 ^oC	4.7%	200 ^oC for 12h	7

References:

1. G. E. Eperon, G. M. Paternò, R. J. Sutton, A. Zampetti, A. A. Haghighirad, F. Cacialli, H. J. Snaith, *J. Mater. Chem. A,* 2015, **3**, 19688-19695.

2. P. F. Luo, W. Xia, S. W. Zhou, L. Sun, J. G. Cheng, C. X. Xu, Y. W. Lu, *J. Phys. Chem. Lett.* 2016, **7**, 3603−3608.

3. T. S. Ripolles, K. Nishinaka, Y. Ogomin, Y. Miyata, S. Hayase, *Solar Energy Materials & Solar Cells*, 2016, **144**, 532–536.

4. A. Swarnkar, A. R. Marshall, E. M. Sanehira, B. D. Chernomordik, D. T. Moore, J. A. Christians, T. Chakrabarti, J. M. Luther, *Science,* 2016, **354**, 92-95.

5. R. J. Sutton, G. E. Eperon, L. Miranda, E. S. Parrott, B. A. Kamino, J. B. Patel, M. T. Hörantner, M. B. Johnston, A. A. Haghighirad, D. T. Moore and H. J. Snaith, *Adv. Energy Mater.,* 2016, **6**. 1502458.

6. R. E. Beal, D. J. Slotcavage, T. Leijtens, A. R. Bowring, R. A. Belisle, W. H. Nguyen, G. F. Burkhard, E. T. Hoke and M. D. McGehee, *J. Phys. Chem. Lett.*, 2016, **7**, 746-751.

7. Q. Ma, S. Huang, X. Wen, M. A. Green and A. W. Y. Ho-Baillie, *Adv. Energy Mater.*, 2016, **6**, 1502202.