Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Enhancing Moisture-tolerance and Photovoltaic Performances for $FAPbI_3$ by Bismuth Incorporation

Yanqiang Hu, [a] Ting Qiu, [a] Fan Bai, [a] Xiaoliang Miao,[a] Shufang Zhang*[a]

This file includes Figure S1-S12 and Table S1-S3:

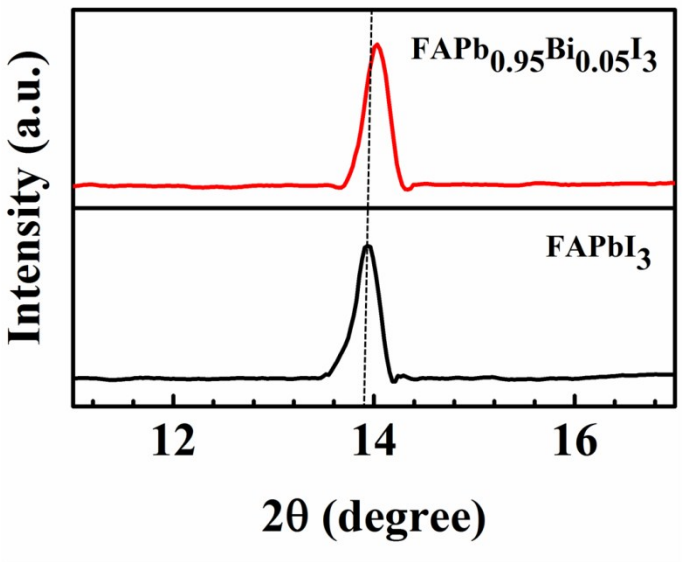

Figure S1. XRD patterns showing a peak shift between the controlled α-$FAPbI_3$ and the $FAPb_{0.95}Bi_{0.05}I_3$ film.

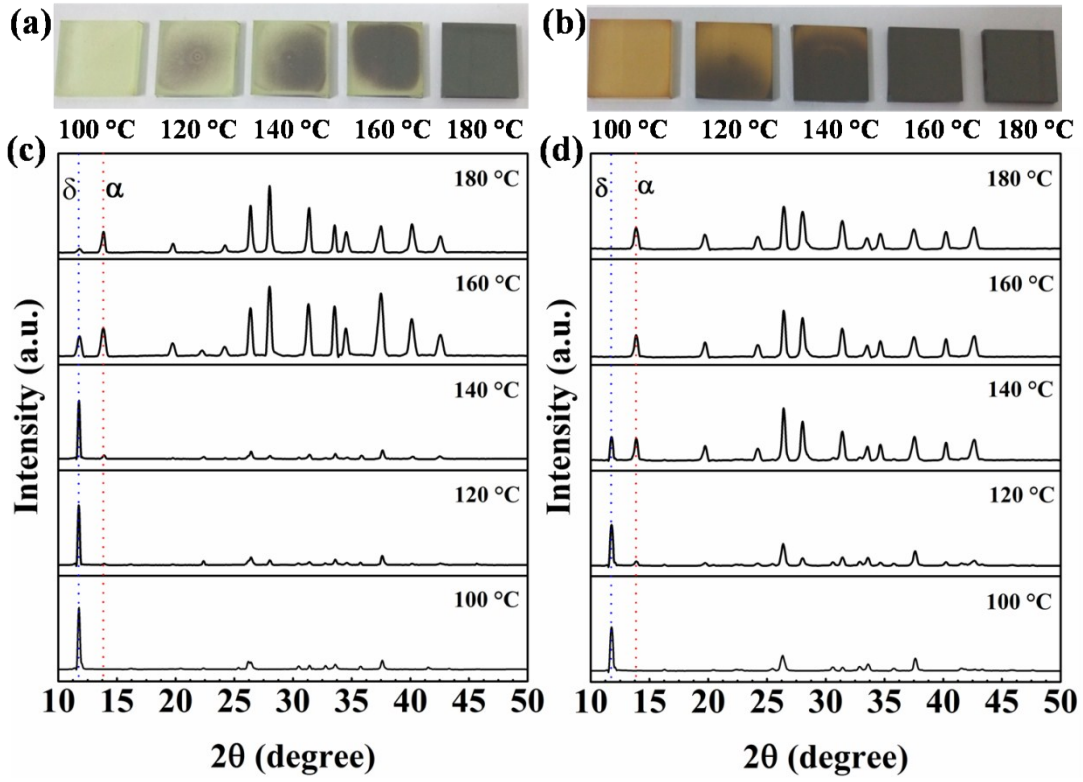

Figure S2. Photograph showing the phase transitions of (a) the controlled $FAPbI_3$ and (b) the $FAPb_{0.95}Bi_{0.05}I_3$ films after heating for 10 min at different temperatures. XRD patterns of (c) $FAPbI_3$ and (d) $FAPb_{0.95}Bi_{0.05}I_3$ films heated at different temperatures for 10 min. δ and α indicate representative peaks for δ-$FAPbI_3$ and α-$FAPbI_3$, respectively.

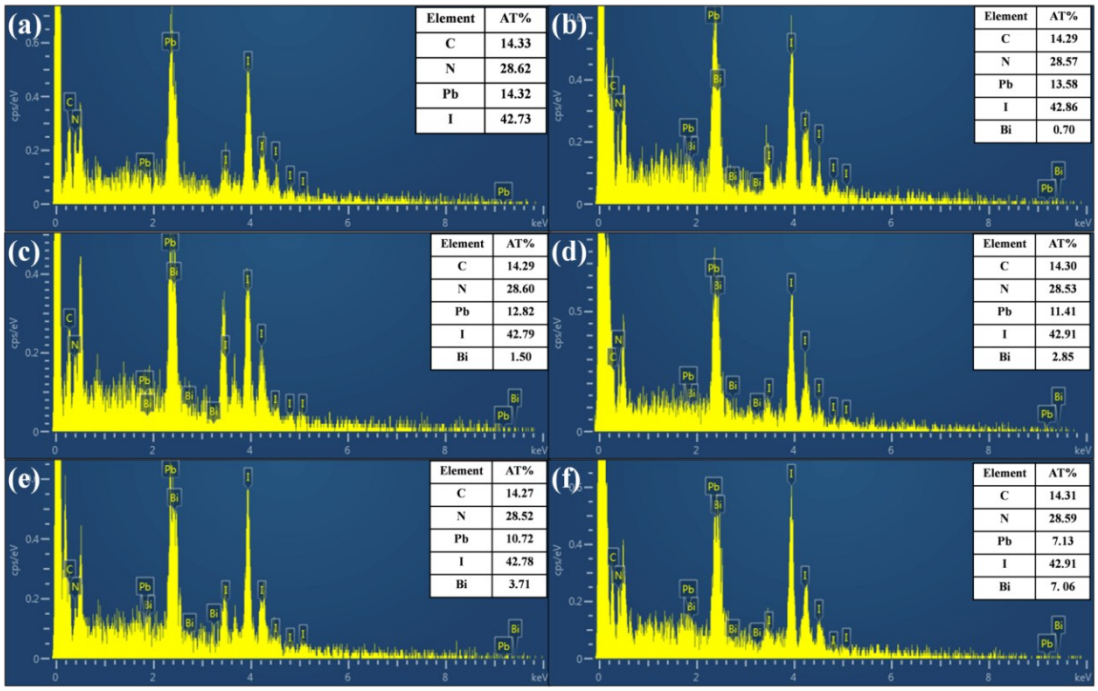

Figure S3. EDS results of the controlled α-$FAPbI_3$ and the Bi-incorporated $FAPb_{1-x}Bi_xI_3$ films. (a) α-$FAPbI_3$, (b) $FAPb_{0.95}Bi_{0.05}I_3$, (c) $FAPb_{0.9}Bi_{0.1}I_3$, (d) $FAPb_{0.8}Bi_{0.2}I_3$, (e) $FAPb_{0.75}Bi_{0.25}I_3$, (f) $FAPb_{0.5}Bi_{0.5}I_3$.

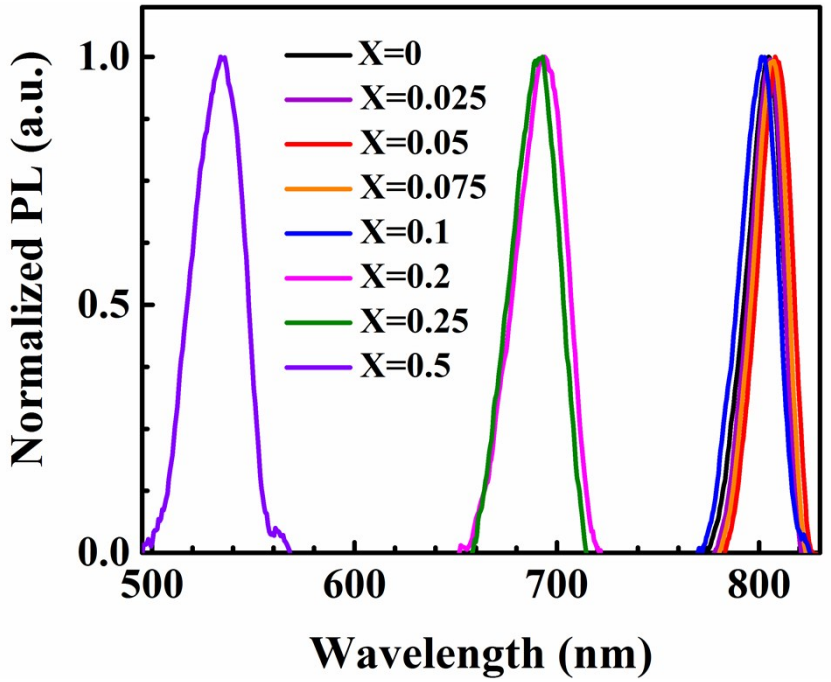

Figure S4. PL spectra of the controlled α-$FAPbI_3$ and the $FAPb_{1-x}Bi_xI_3$ perovskite films.

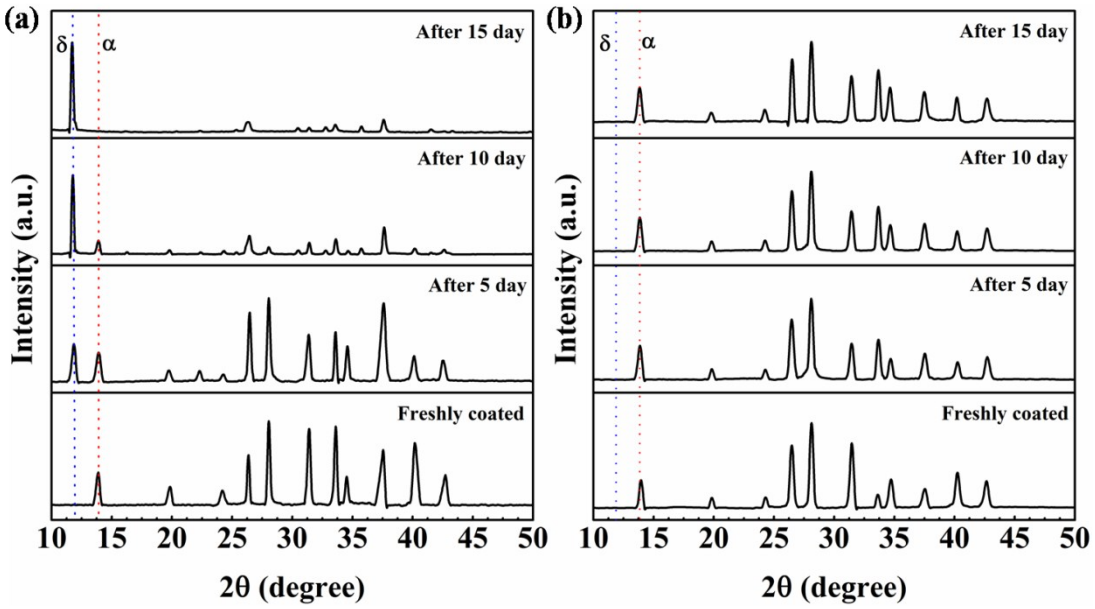

Figure S5. XRD patterns of perovskite films freshly coated and exposed in air for 5 day, 10 day, and 15 day, respectively. (a) The controlled α-$FAPbI_3$ and (b) the $FAPb_{0.95}Bi_{0.05}I_3$ film, respectively.

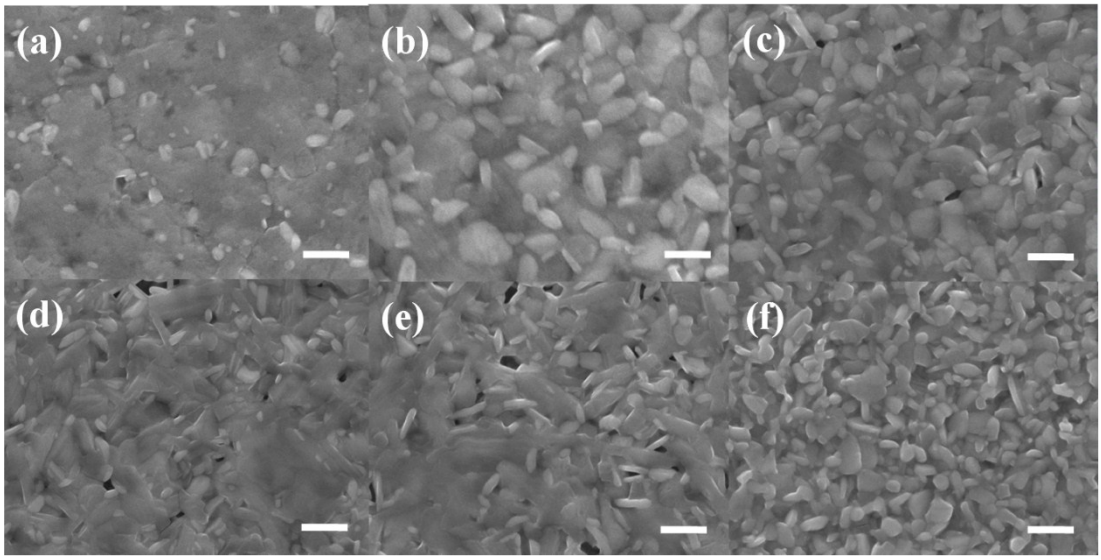

Figure S6. Top-view SEM images of (a) α-$FAPbI_3$, (b) $FAPb_{0.95}Bi_{0.05}I_3$, (c) $FAPb_{0.9}Bi_{0.1}I_3$, (d) $FAPb_{0.8}Bi_{0.2}I_3$, (e) $FAPb_{0.75}Bi_{0.25}I_3$, (f) $FAPb_{0.5}Bi_{0.5}I_3$ capping layers on compact TiO_2 (c-TiO_2) layer-coated FTO glass. Scale bar: 500 nm.

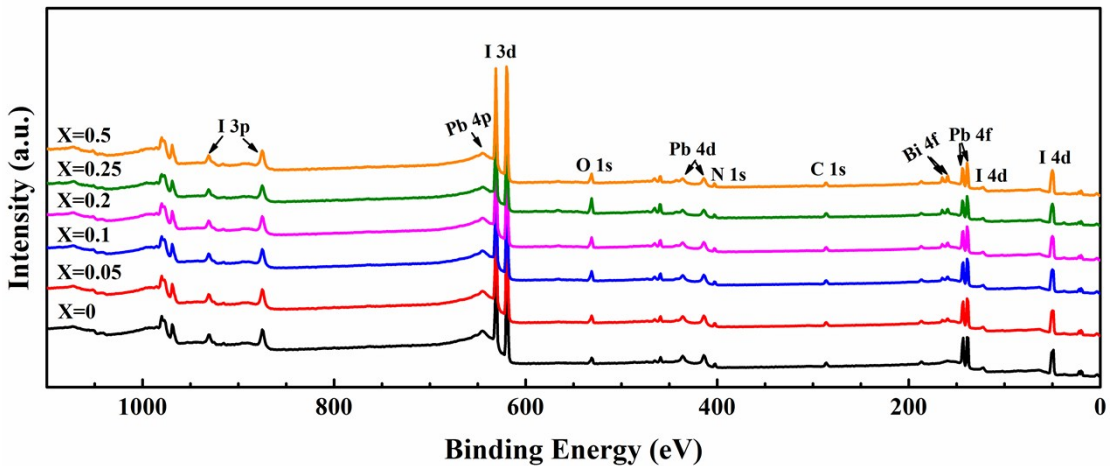

Figure S7. Overview XPS spectra of the controlled α-$FAPbI_3$ and Bi-incorporated $FAPb_{1-x}Bi_xI_3$ films.

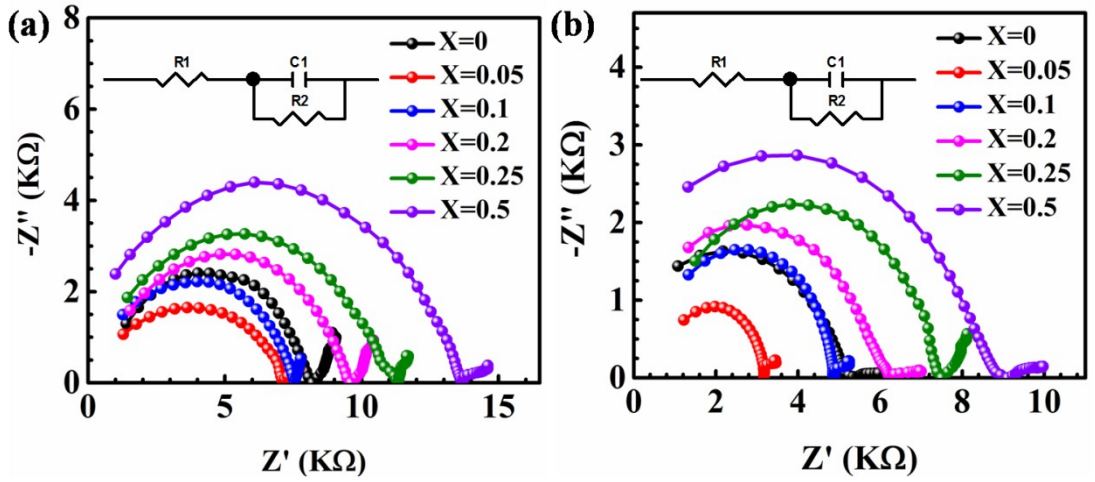

Figure S8. Nyquist plots of the controlled α-$FAPbI_3$ and $FAPb_{1-x}Bi_xI_3$ perovskite films under different conditions (the measured results was shown as dots while the fitted results shown as solid lines). (a) Dark and (b) AM 1.5G illumination. The insets in (a) and (b) is equivalent circuit model, respectively.

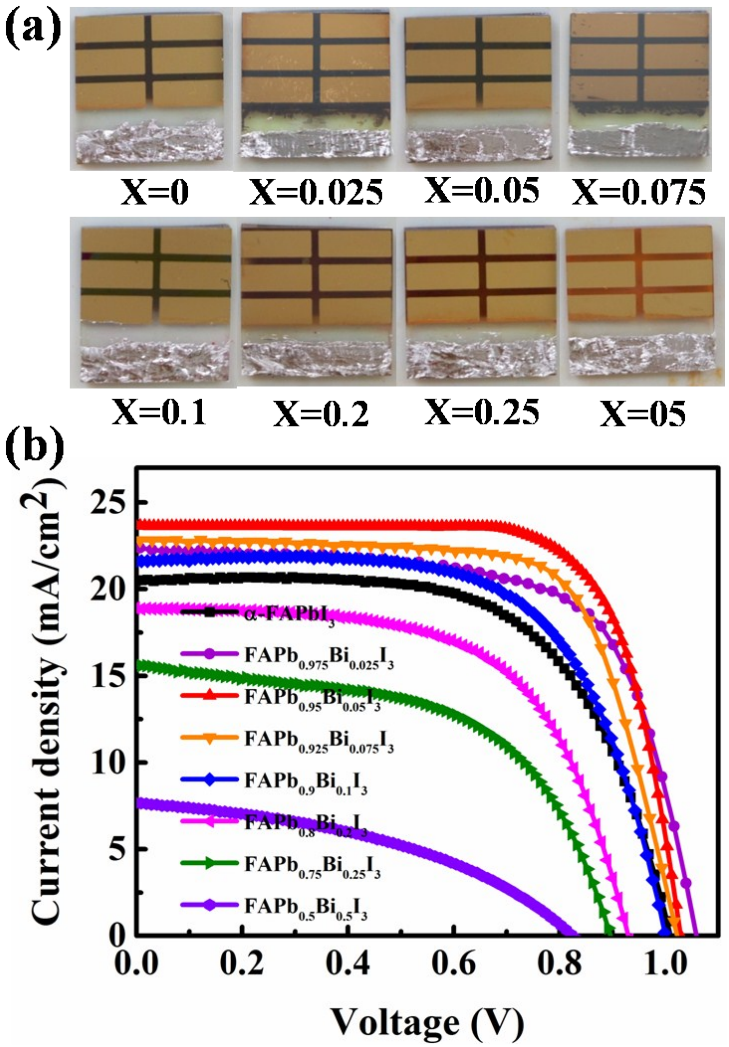

Figure S9. (a) Photographs of solar cells based on the controlled α-$FAPbI_3$ and Bi-incorporated $FAPb_{1-x}Bi_xI_3$ perovskite films. (b) Representative *J-V* curves of solar cells based on the controlled α-$FAPbI_3$ and Bi-incorporated $FAPb_{1-x}Bi_xI_3$.

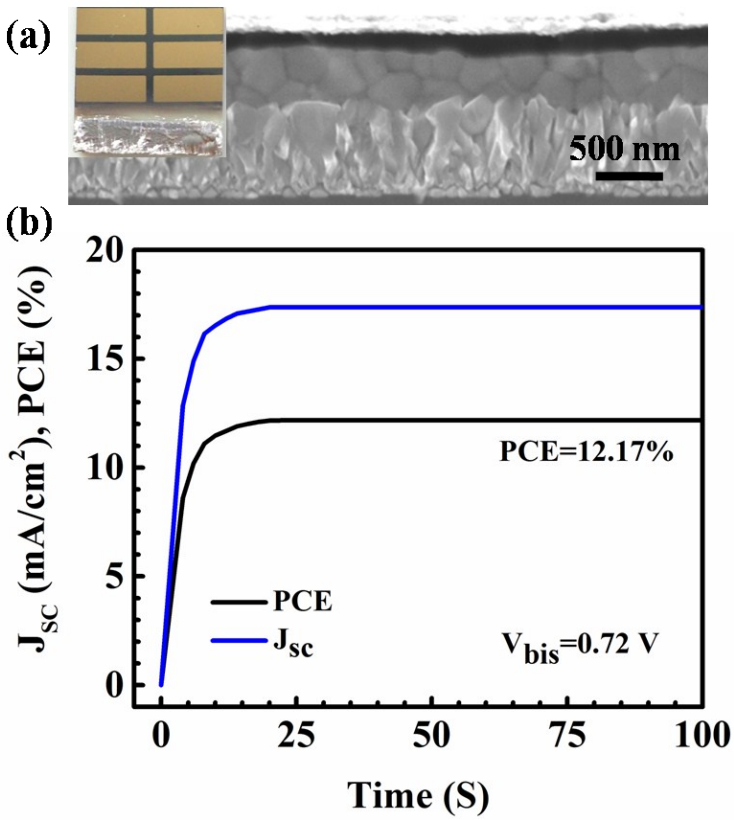

Figure S10. (a) Photograph and corresponding cross-sectional SEM image of based on the controlled α-$FAPbI_3$ solar cells. (b) Photocurrent density and power conversion efficiency as functions of time of the champion solar cell based on the controlled α-$FAPbI_3$ film at the bias of 0.72 V.

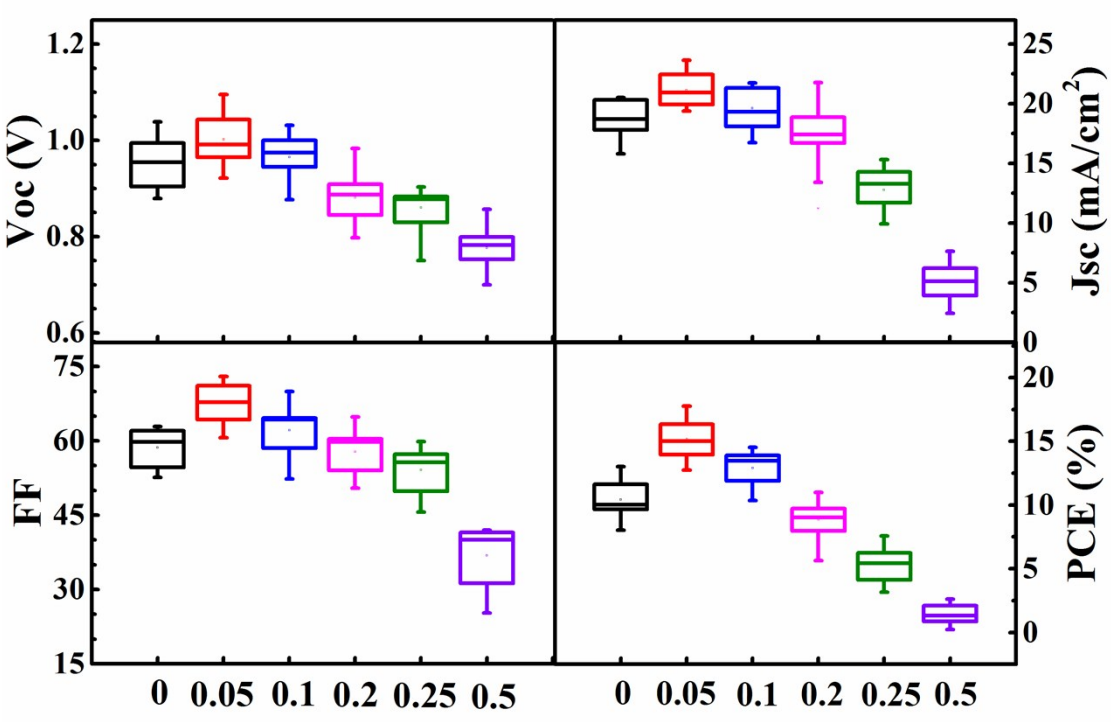

Figure S11. Photovoltaic parameter statistics of the solar cells based on the controlled α-$FAPbI_3$ and Bi-incorporated $FAPb_{1-x}Bi_xI_3$ perovskites.

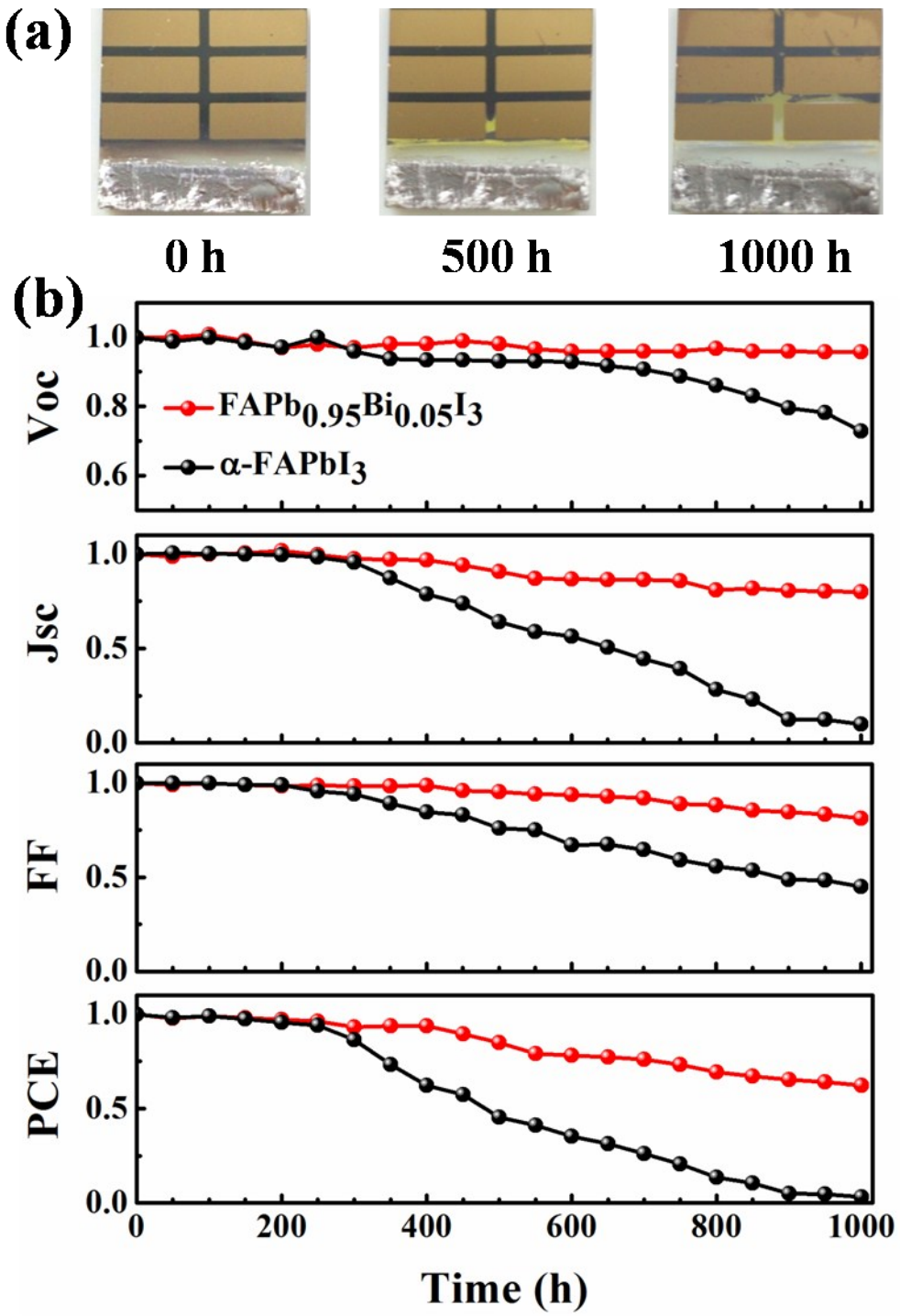

Figure S12. (a) Photographs of solar cell based on the controlled α-$FAPbI_3$ film while exposed in air for 0h, 500h, and 1000 h. (b) Normalized *J*sc, *V*oc, *FF*, and PCE for pure α-$FAPbI_3$ and $FAPb_{0.95}Bi_{0.05}I_3$ planar-architecture perovskite solar cells without encapsulation.

Table S1. The corresponding atomic percentages of the controlled α-$FAPbI_3$ and $FAPb_{1-x}Bi_xI_3$ films got from XPS spectra.

Sample / Element	X=0	X=0.05	X=0.1	X=0.2	X=0.25	X=0.5
C	14.287%	14.265%	14.301%	14.279%	14.312%	14.290%
N	28.653%	28.597%	28.600%	28.634%	28.593%	28.573%
Pb	14.301%	13.569%	12.862%	11.427%	10.703%	7.210%
I	42.759%	42.849%	42.806%	42.799%	42.817%	42.759%
Bi	0	0.720%	1.431%	2.861%	3.575%	7.168%

Table S2. The extracted equivalent circuit element parameters of series of devices based on pure α-$FAPbI_3$ and $FAPb_{1-x}Bi_xI_3$ films under different conditions.

Condition	R	X=0	X=0.05	X=0.1	X=0.2	X=0.25	X=0.5
Dark	Rsh (KΩ)	1.40	1.29	1.27	1.54	1.44	1.01
	Rct (KΩ)	8.20	7.12	7.55	9.61	11.32	13.67
Light	Rsh (KΩ)	1.08	1.22	1.33	1.33	1.49	1.32
	Rct (KΩ)	5.42	3.17	4.86	6.28	7.50	9.11
Δ Rct $[(R_{dark}-R_{light})/R_{dark}]$		33.90%	55.48%	35.63%	34.65%	33.75%	33.36%

Table S3. Photovoltaic parameters of solar cell devices based on the controlled α-$FAPbI_3$ and $FAPb_{1-x}Bi_xI_3$ perovskites.

Perovskite	Voc [V]	Jsc [mA/cm^2]	FF	PCE [%]
α-$FAPbI_3$	1.01	20.50	62.86	13.02
$FAPb_{0.95}Bi_{0.025}I_3$	1.05	22.38	67.62	15.89
$FAPb_{0.95}Bi_{0.05}I_3$	1.03	23.65	72.99	17.78
$FAPb_{0.95}Bi_{0.075}I_3$	1.02	22.81	70.79	16.47
$FAPb_{0.9}Bi_{0.1}I_3$	1.00	21.60	64.72	13.98
$FAPb_{0.8}Bi_{0.2}I_3$	0.93	18.87	60.80	10.67
$FAPb_{0.75}Bi_{0.25}I_3$	0.89	15.30	55.69	7.58
$FAPb_{0.5}Bi_{0.5}I_3$	0.82	7.65	41.50	2.60