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

Supporting Information

Band alignment of Pb-Sn mixed triple cation perovskites for inverted solar cells with negligible hysteresis

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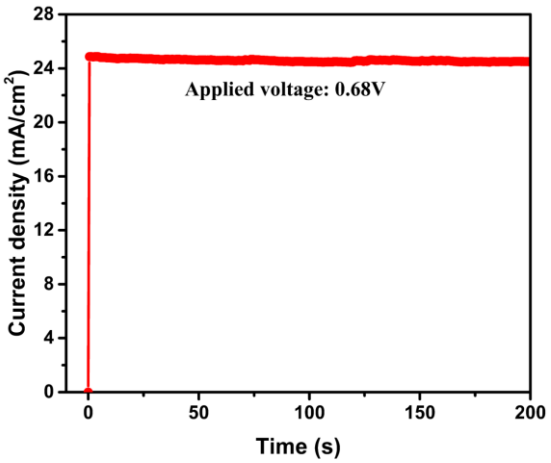


Figure S1. The steady-state photocurrent output of the $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ (x = 0.336) PSCs with an applied voltage of 0.68 V at the maximum power point.

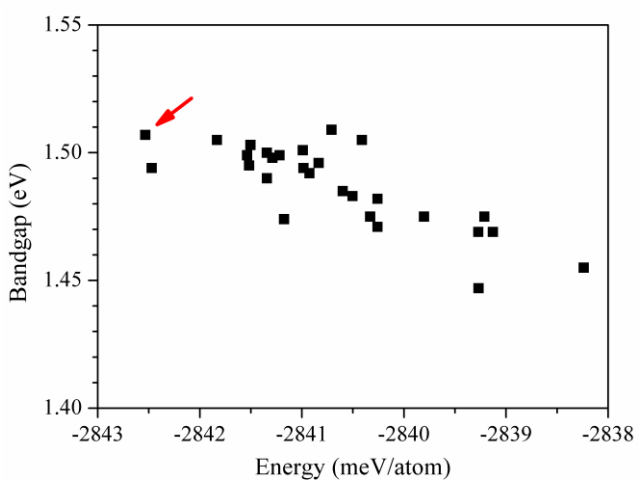


Figure S2. Calculated bandgaps and total energies of $FrPbI_{2.48}Br_{0.52}$ with different I/Br configurations. The one marked by red arrow indicate the I/Br configuration that has the lowest energy and a reasonable bandgap of 1.51 eV, which was considered as the ground-state I/Br configuration for all calculations.

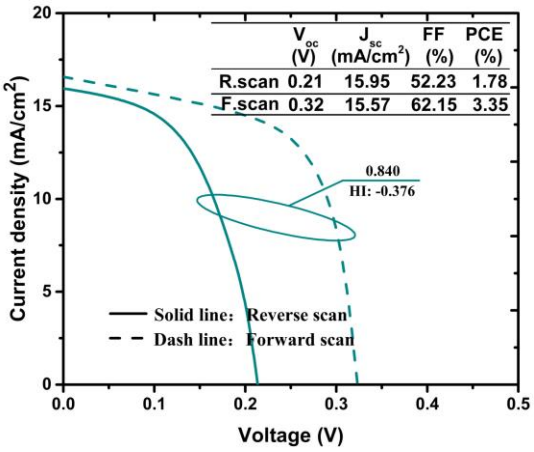


Figure S3. *J-V* curves of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ (x = 0.840) perovskite as light absorbing layer.

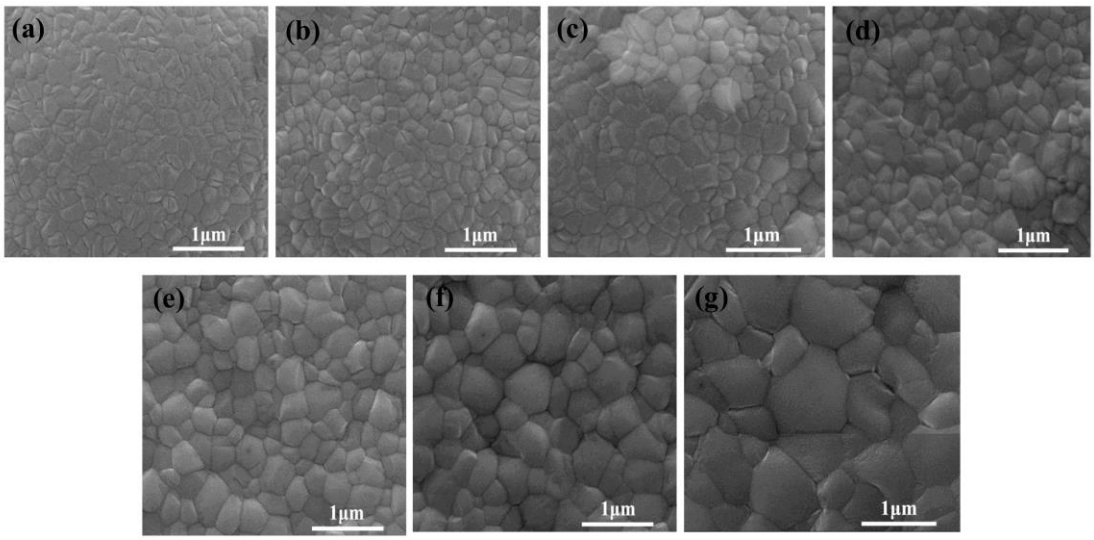


Figure S4. Top-view SEM images of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ perovskite films deposited on PEDOT:PSS with different SnI_2 concentration: a) x = 0.000, b) x = 0.084, c) x = 0.168, d) x = 0.252, e) x = 0.336, f) x = 0.420, g) x = 0.840.

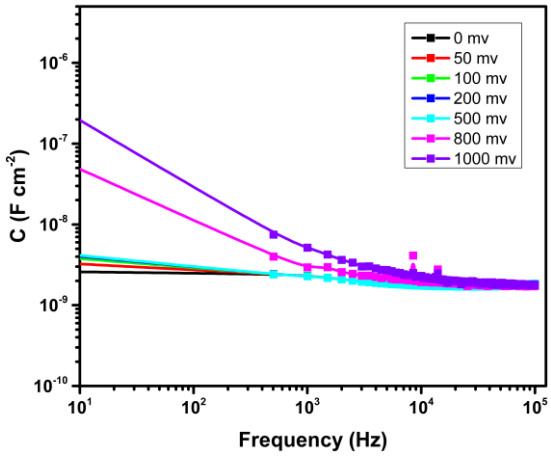
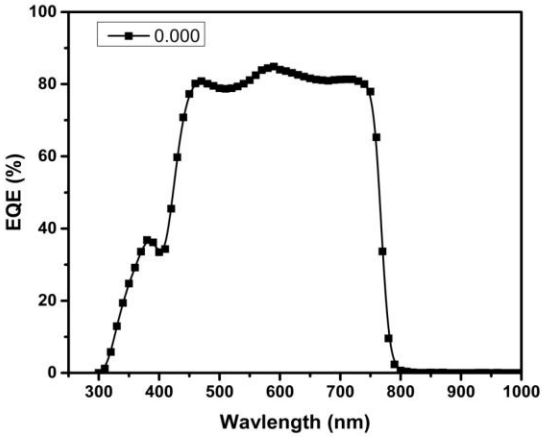
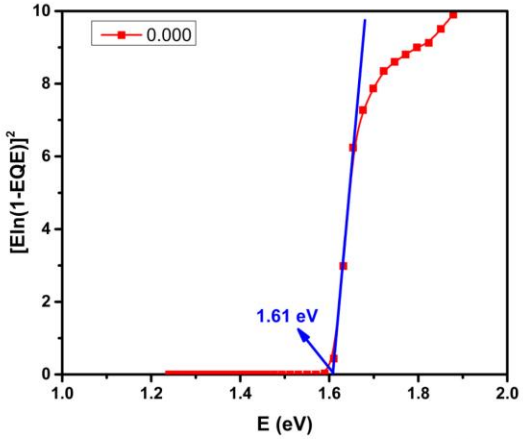
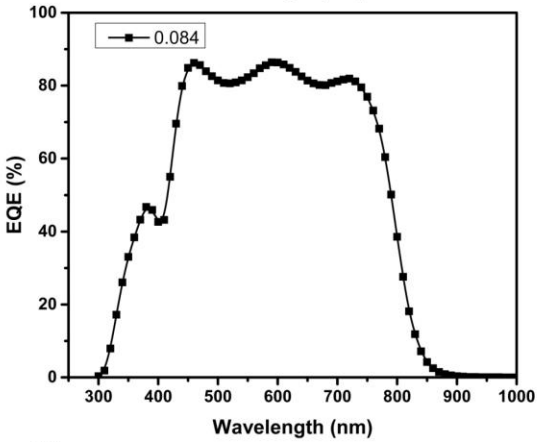
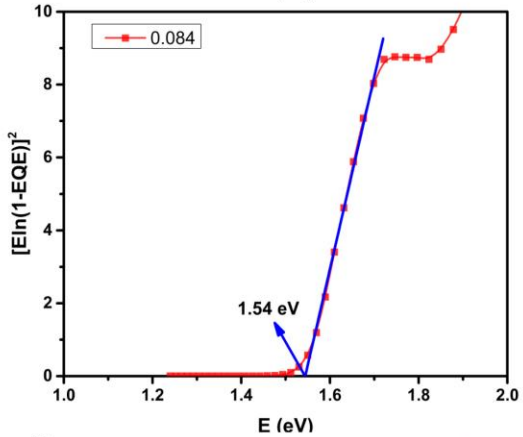


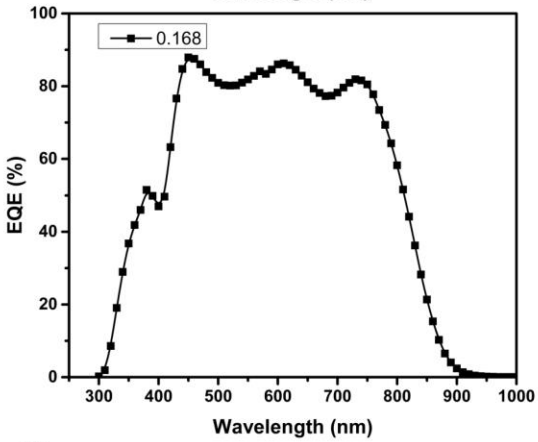
Figure S5. Dark capacitance curve of champion device (x = 0.336) under different bias voltages.

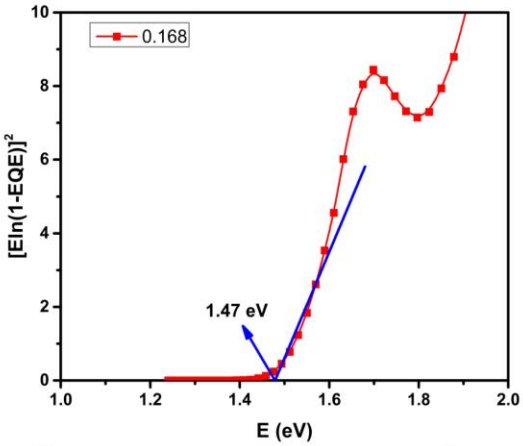

0.000
EQE (%)
Wavlength (nm)

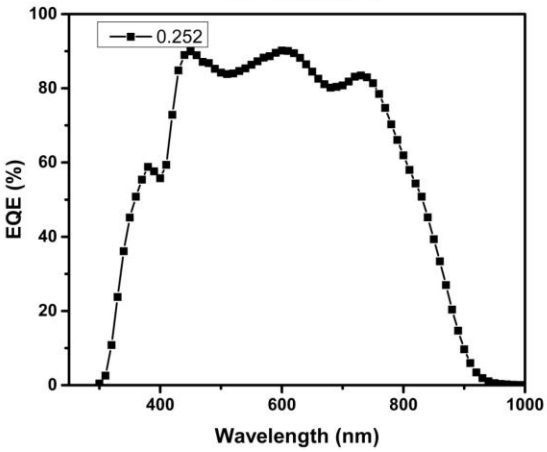

0.000
1.61 eV
[Eln(1-EQE)]²
E (eV)

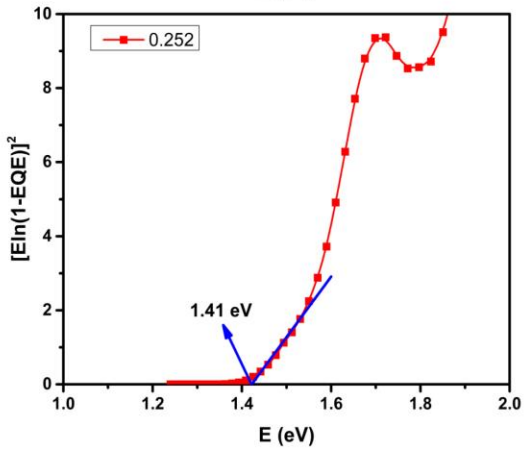

0.084
EQE (%)
Wavelength (nm)


0.084
1.54 eV
[Eln(1-EQE)]²
E (eV)


0.168
EQE (%)
Wavelength (nm)


0.168
1.47 eV
[Eln(1-EQE)]²
E (eV)


0.252
EQE (%)
Wavelength (nm)


0.252
1.41 eV
[Eln(1-EQE)]²
E (eV)

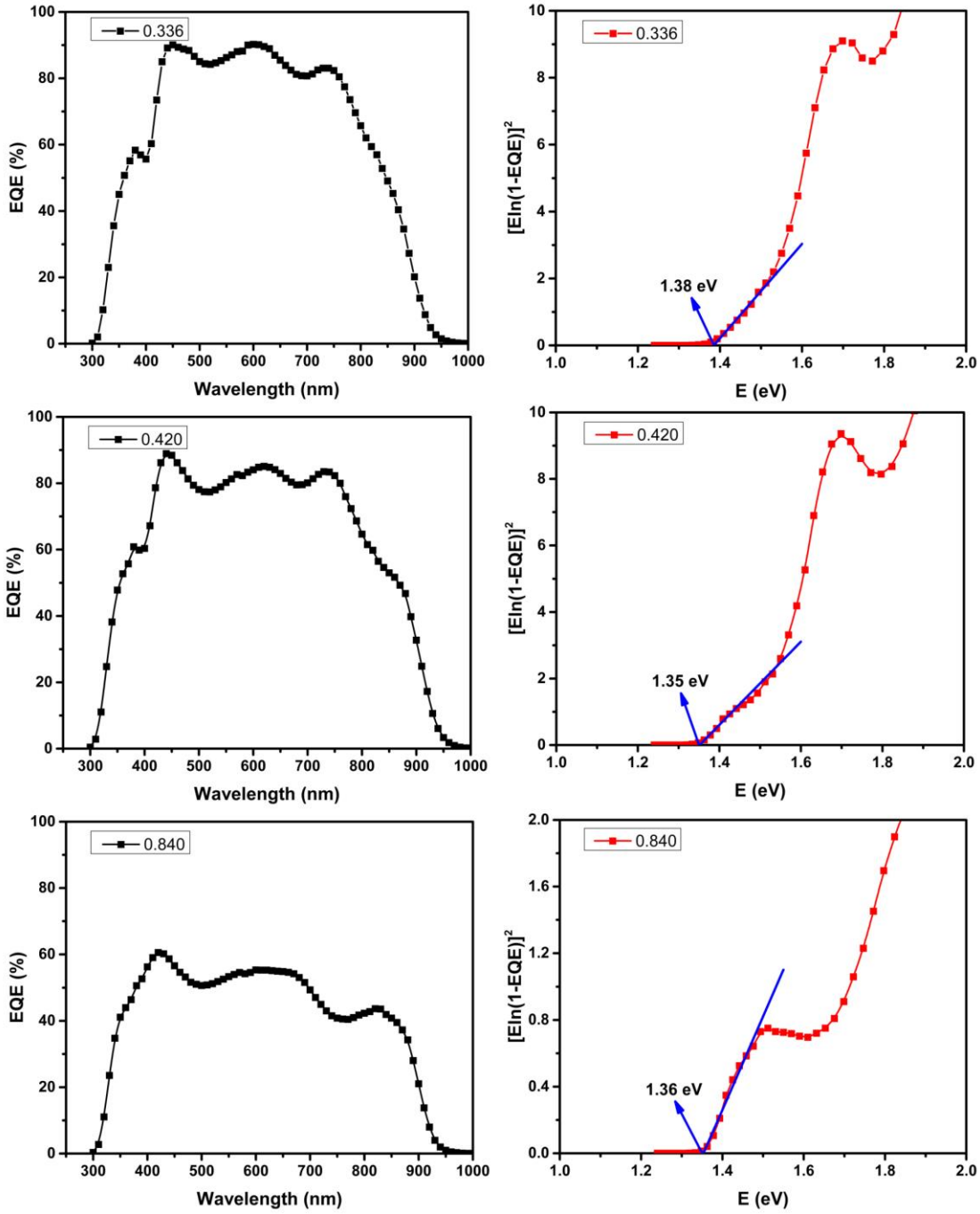


Figure S6. EQE spectra and plots of $[E\times(1-EQE)]^2$ against E of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ perovskite layers.

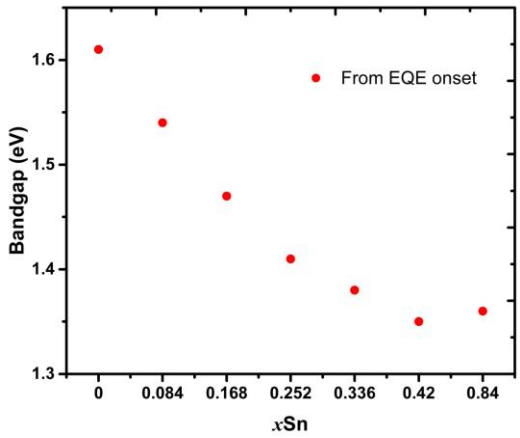


Figure S7. The bandgap values calculated from the onset of the EQE for $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ with increasing Sn contents.

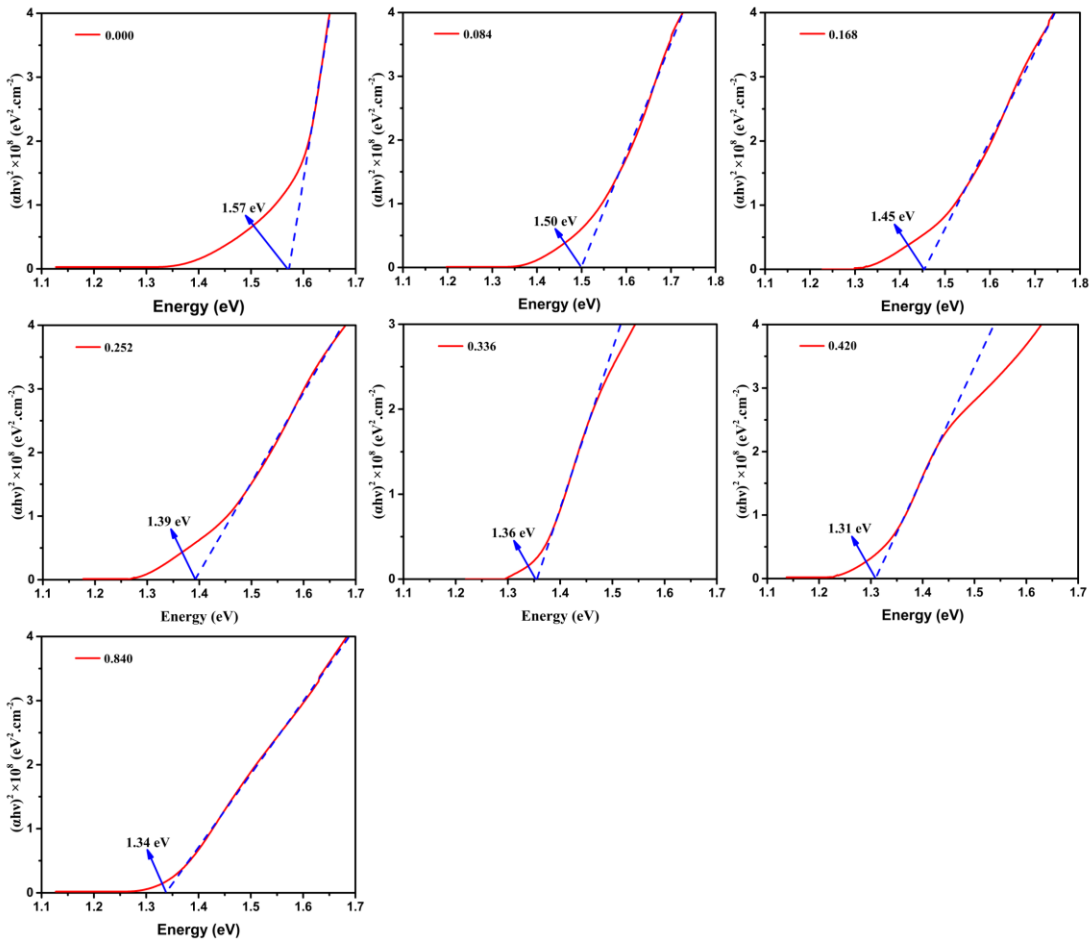


Figure S8. Tauc plots of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ perovskite layers (The slightly calculated bandgap errors are derived from fitting).

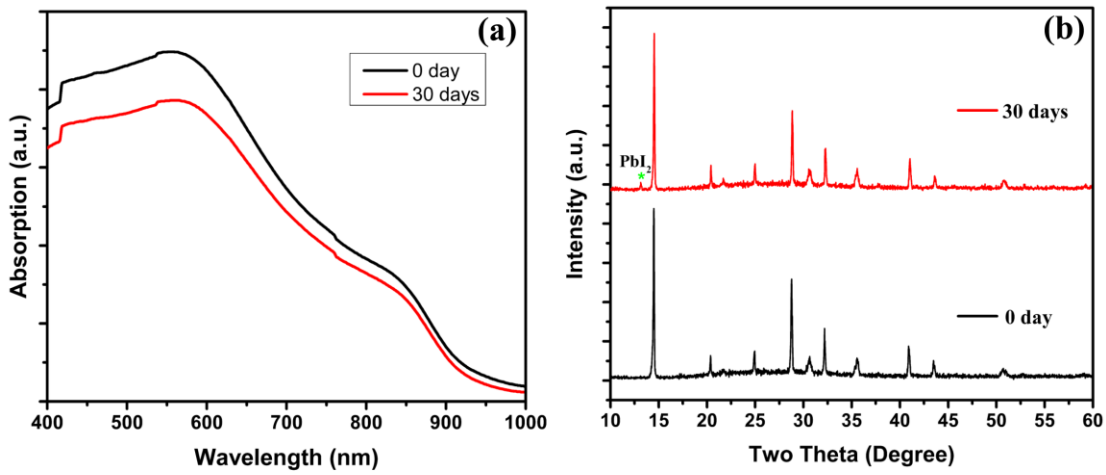


Figure S9. a) Evolution of the absorption spectrum of x = 0.336 samples before and after aging for 30 days in ambient air. b) XRD patterns of x = 0.336 samples before and after aging for 30 days in ambient air.

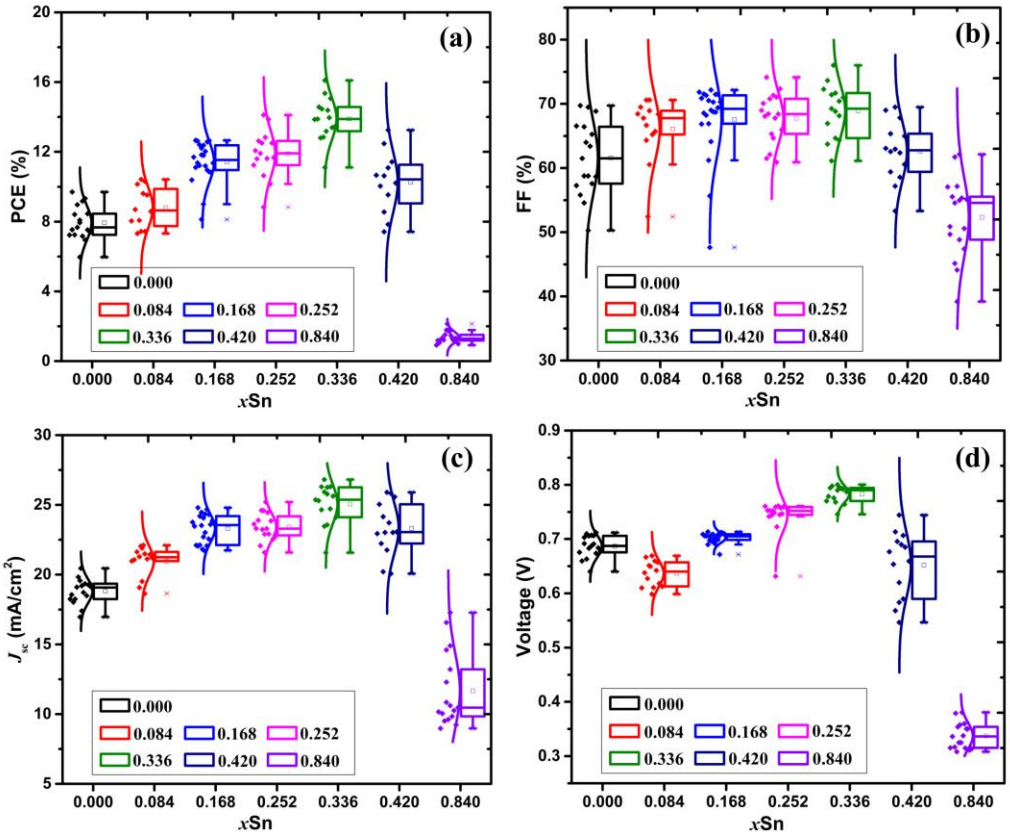


Figure S10. a)-d) Statistical distributions of V_{oc}, J_{sc}, FF and PCE of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ PSCs.

Table S1 Photovoltaic parameters of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ PSCs under different voltage scans.

Different contents of x	Scan direction	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
0.000	Reverse	0.70	19.82	69.75	9.69
	Forward	0.70	19.80	52.03	7.21
0.084	Reverse	0.67	22.10	70.31	10.41
	Forward	0.66	21.72	62.02	8.87
0.168	Reverse	0.71	24.79	72.18	12.65
	Forward	0.70	24.38	66.24	11.27
0.252	Reverse	0.76	25.20	74.15	14.11
	Forward	0.75	24.92	70.09	12.98
0.336	Reverse	0.80	26.59	76.01	16.10
	Forward	0.79	26.45	75.45	15.76
0.420	Reverse	0.74	25.90	69.51	13.25
	Forward	0.72	25.73	65.45	12.10
0.840	Reverse	0.21	15.95	52.23	1.78
	Forward	0.32	15.57	62.15	3.35

Table S2. The measured J_{sc} of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ PSCs from *J-V* curves and the corresponding integrated J_{sc} from EQE spectra.

Different contents of x	0.000	0.084	0.168	0.252	0.336	0.420	0.840
I-V J_{sc} (mA/cm^2)	19.82	22.10	24.79	25.20	26.59	25.90	15.95
Integrated J_{sc} (mA/cm^2)	19.02	21.67	24.32	24.96	26.19	25.21	15.30

Table S3. Photogenerated carrier lifetime and detection wavelength of $Cs_{0.05}FA_{0.79}MA_{0.16}Pb_{1-x}Sn_xX_3$ perovskites. Carrier lifetime is calculated by using double-exponential fit.

Different contents of x	0.000	0.252	0.336	0.420
Detection wavelength (nm)	760	840	850	855
Carrier life time (ns)	25.37	9.08	6.82	2.75