Supporting information

Distribution of bromine in mixed iodide-bromide organolead perovskites and its impact on photovoltaic performance

Yang Zhou, Feng Wang, Honghua Fang, Maria Antonietta Loi, Fangyan Xie, Ni Zhao* and Ching-Ping Wong*

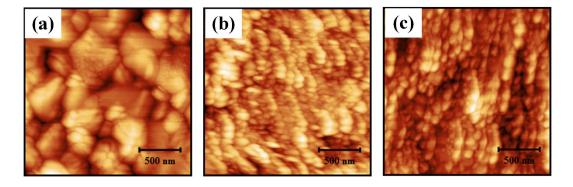


Figure S1. AFM images of MAPb($I_{1-x}Br_x$)₃ films: (a) x=0, (b) x=0.03 and (c) x=0.11.

Table S1. The R_{ms} values of MAPb($I_{1-x}Br_x$)₃ films with x=0, 0.03 and 0.11 derived from the raw data of AFM images.

X	0	0.03	0.12
R _{ms} (nm)	7.72	6.71	4.59

The grain size of the MAPb($I_{1-x}Br_x$)₃ perovskite films is estimated from the full width at half maximum (FWHM) of the XRD peak (2Theta around 30°) according to Scherrer equation $B(2\theta) = \frac{K\lambda}{L\cos\theta}[I]$, where B is the sample's FWHM, θ is diffraction angle, L is the grain size, λ is the wavelength of Cu k α 1 radiation (1.540562A) and K is a constant and for spherical crystals with cubic symmetry this value is 0.94[I]. For the proper determination of the FWHM, the FWHM contributed by Cu k α 2 radiation and the setup is removed. The FWHM contributed by the setup is estimated from the XRD peak (2Theta=30.14°) of the MAPbBr₃ single crystal. The estimated grain sizes are around 200nm for MAPb($I_{1-x}Br_x$)₃ (x=0, 0.03 and 0.11) and are summarized in Table S2.

Table S2. The estimation of grain sizes of the MAPb($I_{1-x}Br_x$)₃ perovskite films with x=0, 0.03, and 0.11.

X	0	0.03	0.11	1 (single crystal)
Peak position 2θ (°)	28.32	28.42	28.54	30.14
FWHM B (mrad)	0.68	0.70	0.77	0.63
Grain size (nm)	220	215	195	NA

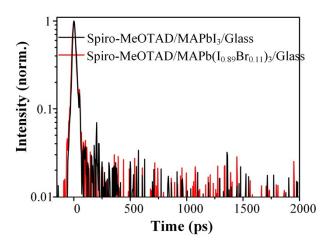


Figure S2. The TRPL decay of HI-aided $MAPb(I_{1-x}Br_x)_3$ (x=0 and 0.11) perovskite films incorporated in between glass and spiro-MeOTAD.

Table S3. Summary of the solar cell performance for MAPb($I_{1-x}Br_x$)₃ perovskite (x=0, 0.03, 0.11, 0.20 and 0.29).

x	Thickness (nm)	J _{sc} (mA/cm ²)	V _{oc} (V)	FF (%)	PCE (%)
0	500	18.42±0.55	0.88±0.01	46.3±3.4	7.5±0.8
	330	21.10±0.30	0.98±0.01	68.5±3.3	14.2±0.6
	240	19.60±0.48	0.96±0.01	58.9±2.0	11.1±0.4
0.03	500	18.96±0.38	0.97±0.01	60.3±2.2	11.2±0.6
0.11	260	18.53±0.36	1.02±0.02	61.9±0.4	11.7±0.8
	340	20.44±0.20	1.00±0.01	59.0±1.8	12.1±0.4
	460	21.55±0.41	1.01±0.02	68.2±0.8	14.8±0.6
	510	22.38±0.28	1.01±0.02	70.3±1.7	15.8±0.6
	570	20.59±0.59	1.01±0.01	61.8±0.3	12.8±0.5
	660	17.99±0.37	1.00±0.01	58.0±0.5	10.4±0.2
0.20	510	19.86±0.35	1.09±0.01	63.7±0.2	13.8±0.6
0.29	510	13.54±0.62	0.92±0.02	36.8±0.9	4.6±0.3

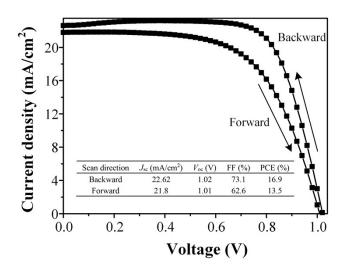


Figure S3. The PV performance of the champion cell prepared from $MAPb(I_{0.89}Br_{0.11})_3$ perovskite.