Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2017

Electronic Supplementary Information

Formamidinium-methylammonium lead iodide perovskite single crystal exhibits exceptional optoelectronic properties and long-term stability

Wen-Guang Li, Hua-Shang Rao, Bai-Xue Chen, Xu-Dong Wang and Dai-Bin Kuang*

MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional Materials, School of Chemistry, Sun Yat-sen University, Guangzhou 510275, P. R. China.

* Corresponding author

Fax: (+86) 20-84113015

Email: kuangdb@mail.sysu.edu.cn

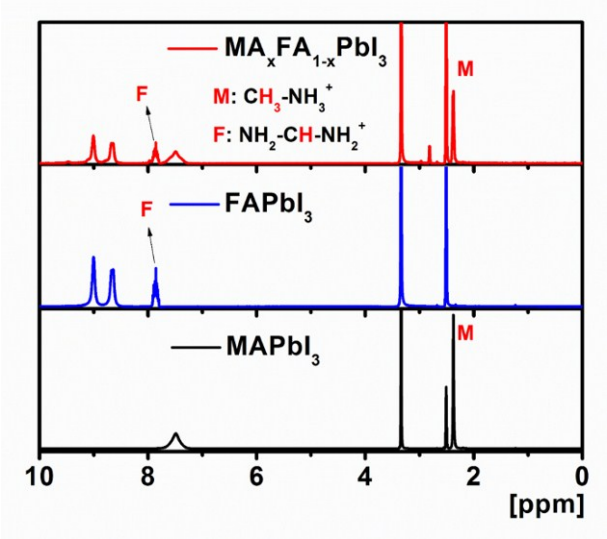

Fig. S1 ^{1}H NMR spectra of $MAPbI_3$, $FAPbI_3$, and the mixed cation perovskite single crystals.

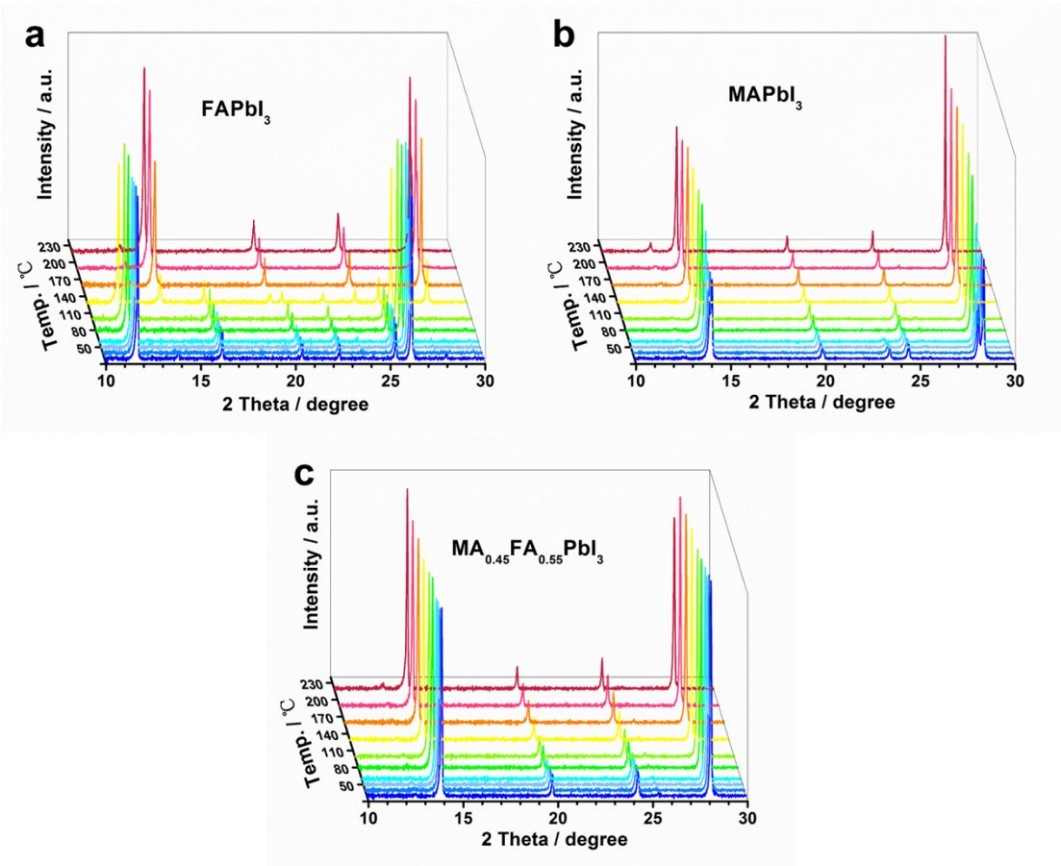

Fig. S2 Temperature-dependent XRD patterns of (a) $FAPbI_3$, (b) $MAPbI_3$, and (c) $MA_{0.45}FA_{0.55}PbI_3$ single crystals ground to powder.

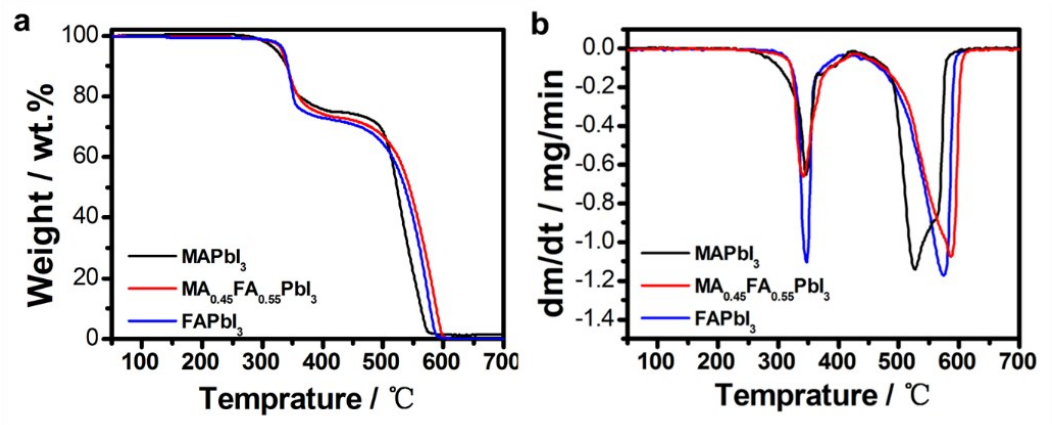

Fig. S3 TGA curves (a) and their corresponding first derivative curves (b) of $MAPbI_3$, $FAPbI_3$, and $MA_{0.45}FA_{0.55}PbI_3$ single crystals ground to powder.

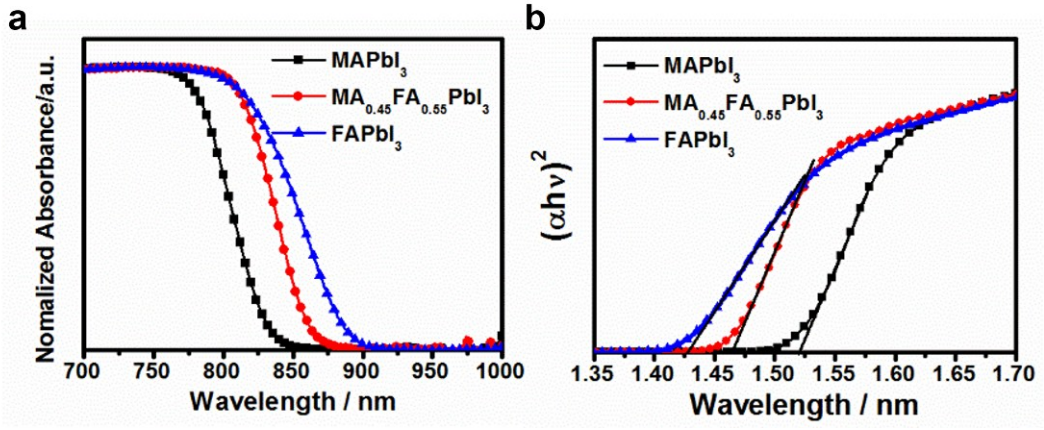

Fig. S4 (a) UV-vis-NIR absorption spectra and (b) Tauc plots to extract the optical bandgaps of $MAPbI_3$, $FAPbI_3$ and $MA_{0.45}FA_{0.55}PbI_3$ single crystals.

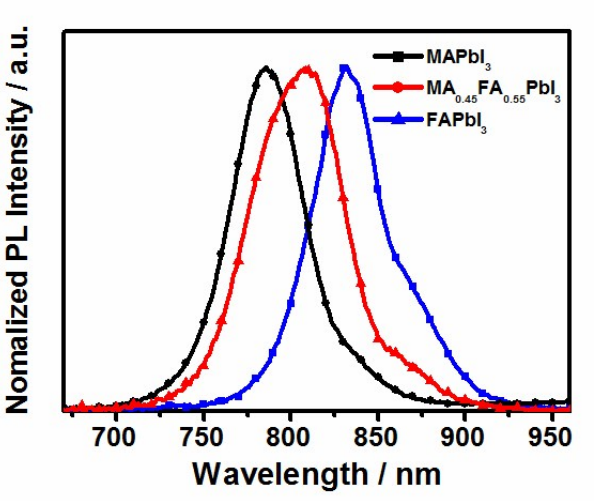

Fig. S5 Photoluminescence spectra of $MAPbI_3$, $FAPbI_3$ and $MA_{0.45}FA_{0.55}PbI_3$ single crystals.

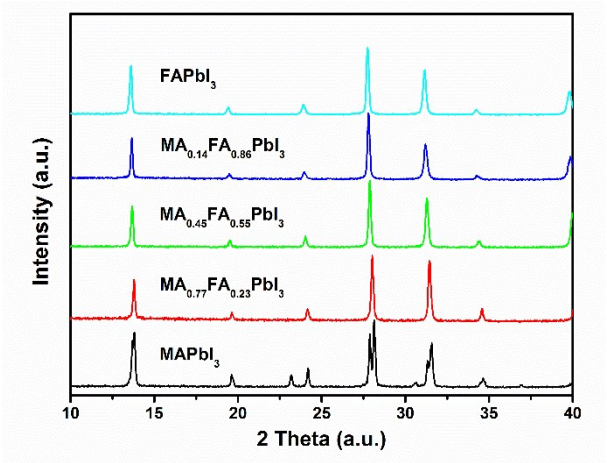

Fig. S6 The powder XRD spectra of the $MA_xFA_{1-x}PbI_3$ single crystals with x = 0, 0.14, 0.45, 0.77, 1.0.

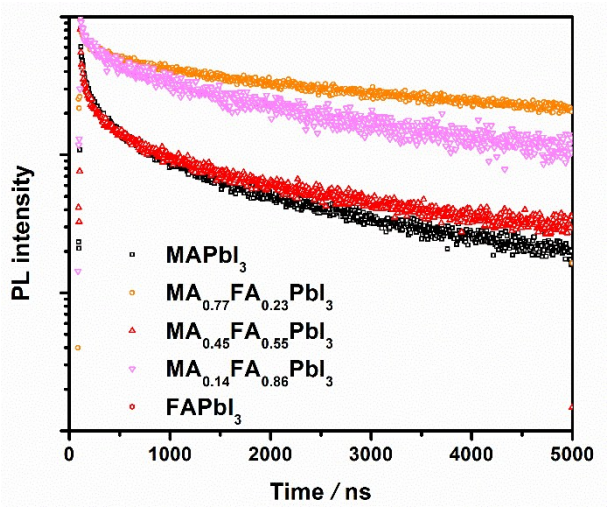

Fig. S7 Time-resolved photoluminescence spectra of the $MA_xFA_{1-x}PbI_3$ single crystals with x = 0, 0.14, 0.45, 0.77, 1.0.

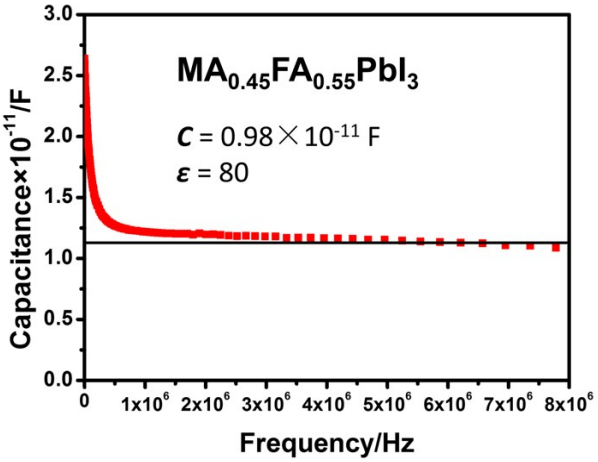

Fig. S8 The frequency dependent capacitance curve for the $MA_{0.45}FA_{0.55}PbI_3$ single crystal.

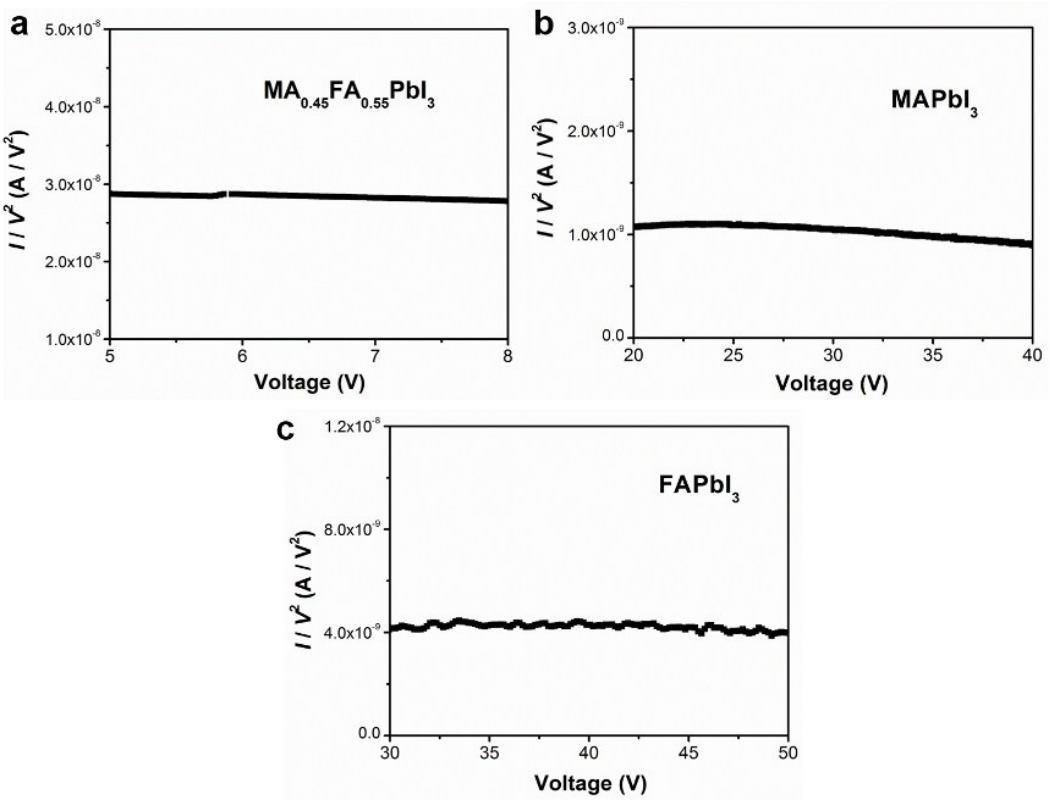

Fig. S9 I/V^2-V plots of the dark I-V curves in Child's region. (a) $MA_{0.45}FA_{0.55}PbI_3$, (b) $MAPbI_3$ and (c) $FAPbI_3$ single crystal.

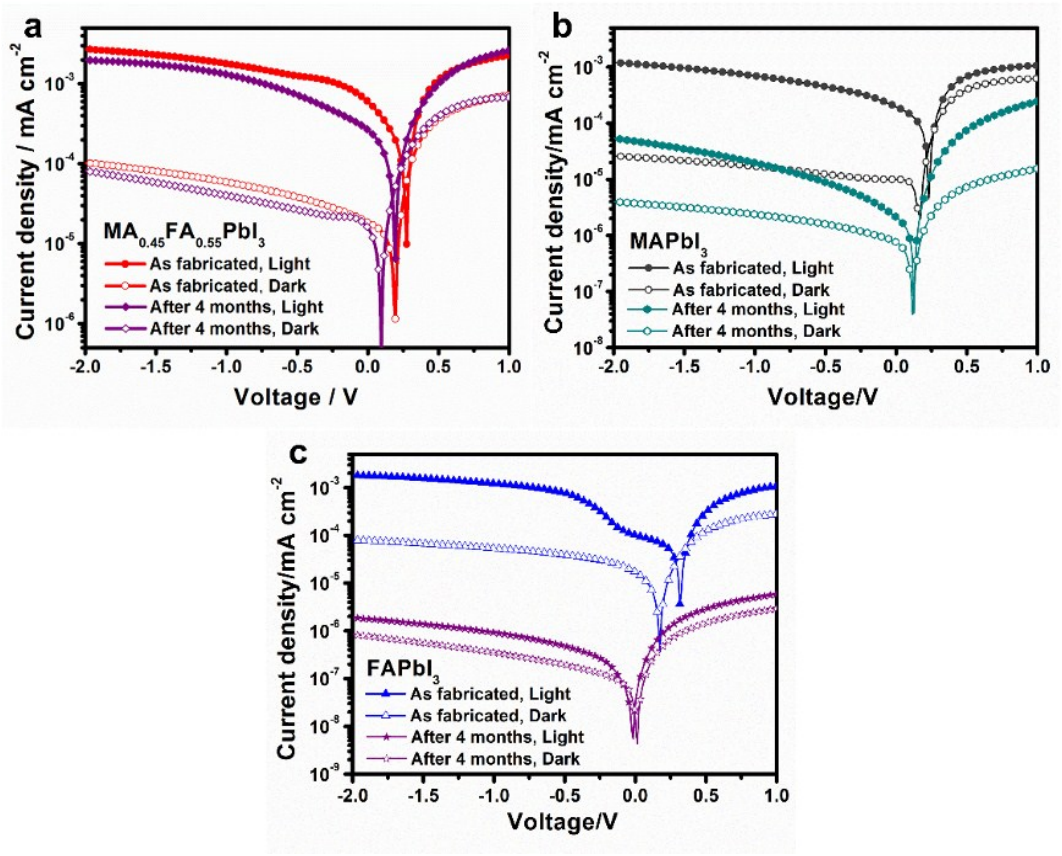

Fig. S10 Dark current and photocurrent curves of the (a) $MA_{0.45}FA_{0.55}PbI_3$, (b) $MAPbI_3$ and (c) $FAPbI_3$ single-crystal photodetectors and the same devices after stored in an opaque desiccator (RH ~10 %) for 4 months. The photocurrent was measured under illumination of ~20 μW cm^{-2} from 870 nm LED.

Table S1 Fluorescence lifetime and corresponding intensities derived from the fitting results of the photoluminescence decay curves.

	τ_1/ns	Rel/%	τ_2/ns	Rel/%	τ_{total}/ns
$MAPbI_3$	70	15%	1053	85%	906
$MA_{0.77}FA_{0.23}PbI_3$	51	4%	1162	96%	1118
$MA_{0.45}FA_{0.55}PbI_3$	124	4%	2205	96%	2122
$MA_{0.14}FA_{0.86}PbI_3$	61	12%	1122	88%	995
$FAPbI_3$	131	6%	1714	94%	1619

Table S2 The properties comparison of $MA_xFA_{1-x}PbI_3$ single crystals with literatures.

	I.	μ ($cm^2\ s^{-1}\ V^{-1}$)	n_c (cm^{-3})	n_t (cm^{-3})	τ (μs) (from PL)	$\tau_{1\ SUN}$ (μs) (from TPV)	L_D (μm) (from PL)	L_D (μm) (from TPV)	reference
$MAPbI_3$	1×10^{-8}	2.5	2×10^{10}	$3.3 \pm 0.3 \times 10^{10}$	0.022, 1.032	-	2, 8	-	*Science*, 2015, **347**, 519-522
$MAPbI_3$	-	164 ± 25	$9 \pm 2 \times 10^9$	3.6×10^{10}	-	82 ± 5	-	175 ± 25	*Science*, 2015, **347**, 967-970.
$MAPbI_3$	-	167 ± 35	-	$1.80 \pm 1.07 \times 10^9$	-	-	-	-	*J. Am. Chem. Soc*., 2016, **138**, 9409-9412.
$MAPbI_3$	-	39.6	-	6.0×10^8	-	-	-	-	*Adv. Mater*., 2016, **28**, 9204-9209
α-$FAPbI_3$	1.1×10^{-7}	4.4	1.5×10^{11}	6.2×10^{11}	0.032, 0.484		0.5, 2.2	-	*Adv. Mater.*, 2016, **28**, 2253-2258
α-$FAPbI_3$	2.2×10^{-8}	35 ± 7	3.9×10^9	1.1×10^{10}	0.032, 0.484	-	1.7, 6.6	-	*ACS Energy Lett*., 2016, **1**, 32-37
α-$FAPbI_3$	1.8×10^{-8}	40 ± 5	2.8×10^9	1.34×10^{10}	-	-	-	-	*Adv. Optical Mater.*, 2016, **4**, 1829-1837
$MAPbI_3$	1.1×10^{-8}	65 ± 6	1.0×10^9	1.1×10^{10}	0.070, 0.906	80	3.4, 12.3	115	Present work
α-$FAPbI_3$	2.2×10^{-8}	150 ± 15	9.5×10^8	8.2×10^9	0.131, 1.619	37	7.1, 25.0	118	Present work
$MA_{0.45}FA_{0.55}PbI_3$	1.7×10^{-7}	271 ± 60	3.9×10^9	2.6×10^9	0.124, 2.122	93	9.29, 38.4	254	Present work