Supporting Information

Thermal Quenching and Dose Studies of X-ray Luminescence in Single

Crystals of Halide Perovskites

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Figure S1. X-ray diffraction (XRD) pattern of a) MAPbCl₃, b) MAPbBr₃, c) MAPbI₃, and d) CsPbBr₃ powders of single crystals and simulation from published single crystal information.¹⁻⁴ The extra peaks in MAPbI₃ may come from the side product after decomposition in ambient.

Single crystal X-ray diffraction (SCXRD)

Here we demonstrate MAPbBr₃ as an example to show our perovskite crystal samples have the single-crystal quality. The MAPbBr₃ sample was prepared by cleaving a small piece (orange shard with the size of 300 – 500 micrometers) from the as-grown crystal. The SCXRD machine was Bruker Smart APEXII SC-XRD equipped with Mo K_a radiation ($\lambda =$ 0.71 Å). The absorption correction, model construction and model refinement were done with SADABS, SHEXT and SHELEX-2014 software package, respectively. The detail of crystal structure from our sample can be found in our Crystallographic Information File (MAPbBr₃.cif) in supporting information. Our results matches very well with the published MAPbBr₃ data.²

Emprirical Formula	CH ₆ NPbBr ₃
Wavelength, Å	0.71073
Formula Weight, g/mol	478.99
Temperature, K	296(2)
Crysatl system	Cubic
Space group	Pm3m
a, Å	5.932(2)
b, Å	5.932(2)
c, Å	5.932(2)
$\alpha = \beta = \gamma, \circ$	90
Volume, Å ³	208.7(3)
Z	1
Density (calculated), g/cm ³	3.811
Aborption coefficient, /mm	34.64
F(000)	206
Crystal size, mm ³	0.44 * 0.36 * 0.3
θ range, °	5.96 to 34.64
Index ranges	$-5 \le h \le 8, -9 \le k \le 4, -4 \le l \le 5$
Completeness	100 %
Final R index (all data)	0.0418
Largest diff. peak and hole, e/ $Å^3$	1.682, -1.676

Table S1. Crystallograppic data for α -MAPbBr₃ at ambient pressure

Proof of Bi³⁺ doping in MAPbBr₃



Figure S2. Photoluminescence spectra of undoped, 1/100 and 1/10 Bi-doped MAPbBr₃ at room temperature. The absence of PL in 1/100 and 1/10 doped samples verify the Bi doping.

Table 52. Four-point probe measurement for BF-doped WAT obly	
Sample	Sheet resistance
Undoped	No reading (too large)
1/100	$4.2 \pm 1.0 \text{ M}\Omega/\text{sqr}$
1/10	$0.208 \pm 0.082 \text{ M}\Omega/\text{sqr}$

Table S2. Four-point probe measurement for Bi-doped MAPbBr₃

The decrease in sheet resistance upon higher Bi concentration also confirms the successful Bi doping.

Thermoluminescence (TL) spectrum of 1/100 Bi-doped MAPbBr₃



Figure. S3. TL spectrum of 1/100 Bi-doped MAPbBr₃. Traps can be determined from the afterglow emission.⁵ Such afterglow partly verifies the possible polaron traps caused by the Bi doping since there is no afterglow in undoped MAPbBr₃.

References

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