

Supplementary Information

Ionic liquid assisted high quality MAPbBr₃ Single Crystal growth for Photodetection Application

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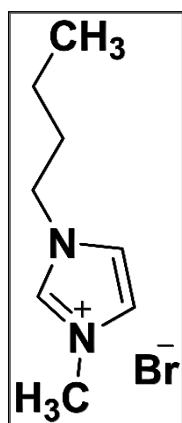


Figure S1. Molecular structure of BMIB IL.

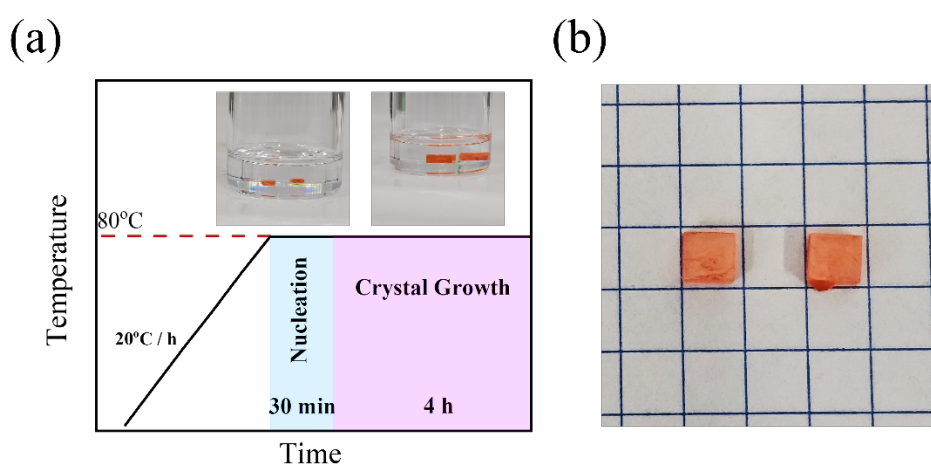


Figure S2. (a) Schematic representation of crystallization rate over time for MAPbBr₃ SCs using ITC method at 80°C. (b) Image of as-grown MAPbBr₃ SCs.

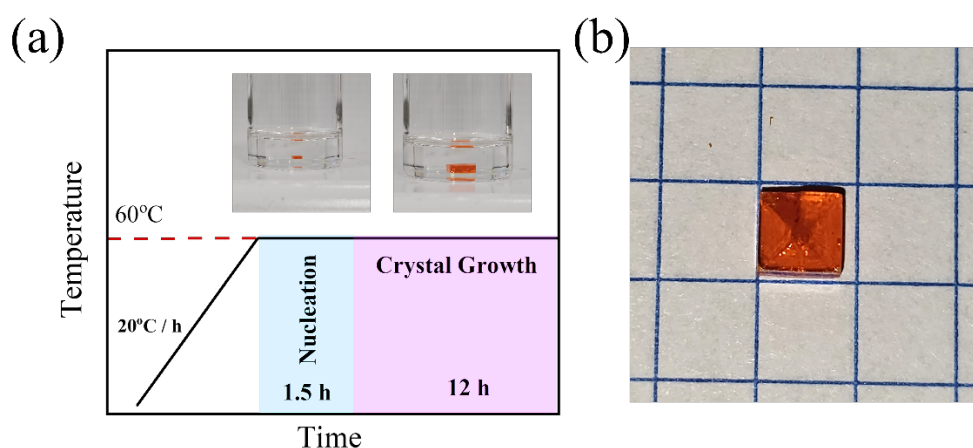


Figure S3. (a) Schematic representation of crystallization rate over time for MAPbBr₃ SCs using ITC method at 80°C. (b) Image of as-grown MAPbBr₃ SC in the presence of BMIB (5 %mol).

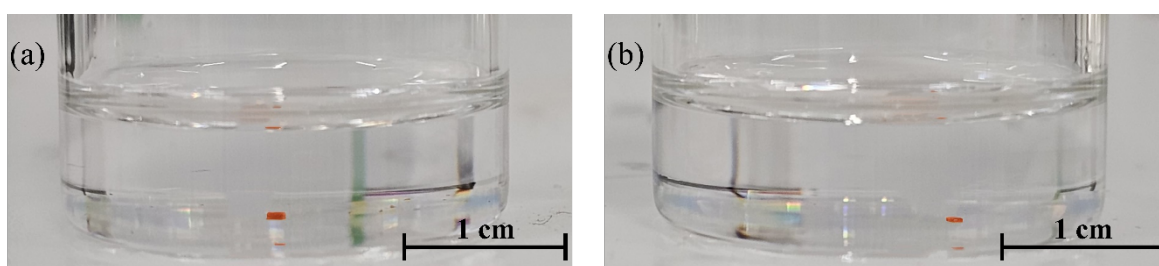


Figure S4. Photographs of MAPbBr₃ solution heated at 60°C for 12 h with (a) 1 mol% and (b) 3 mol% BMIB IL.

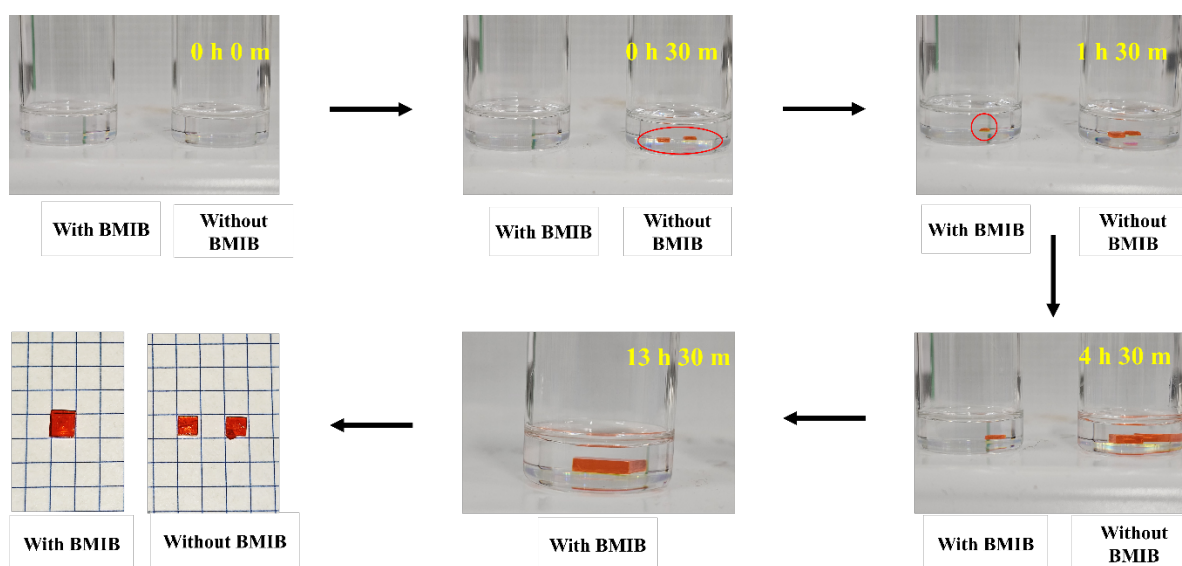


Figure S5. Image of crystallization process without and with 5 mol% BMIB IL at 80°C as a function of time.

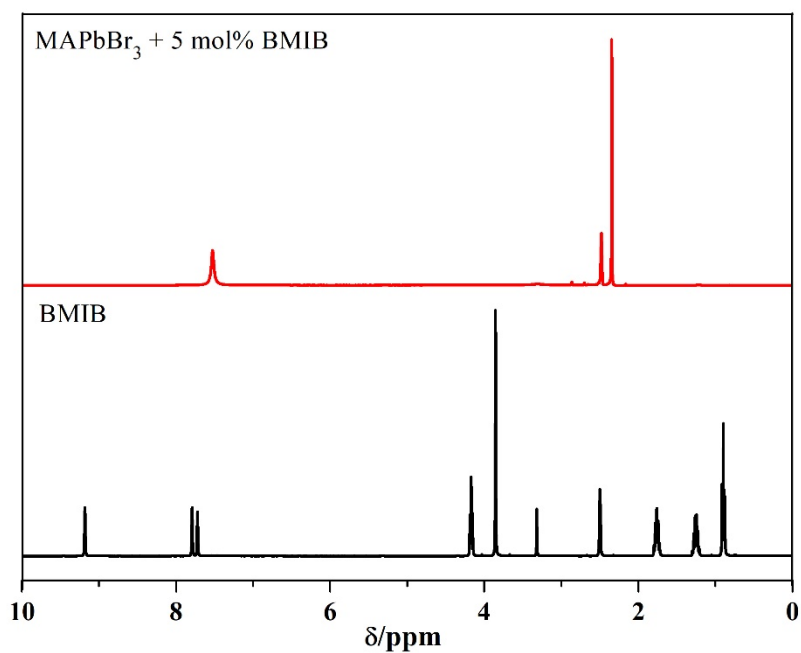


Figure S6. ^1H NMR spectrum of BMIB and MAPbBr₃ crystals with 5 mol% of BMIB measured in DMSO-d₆ solution.

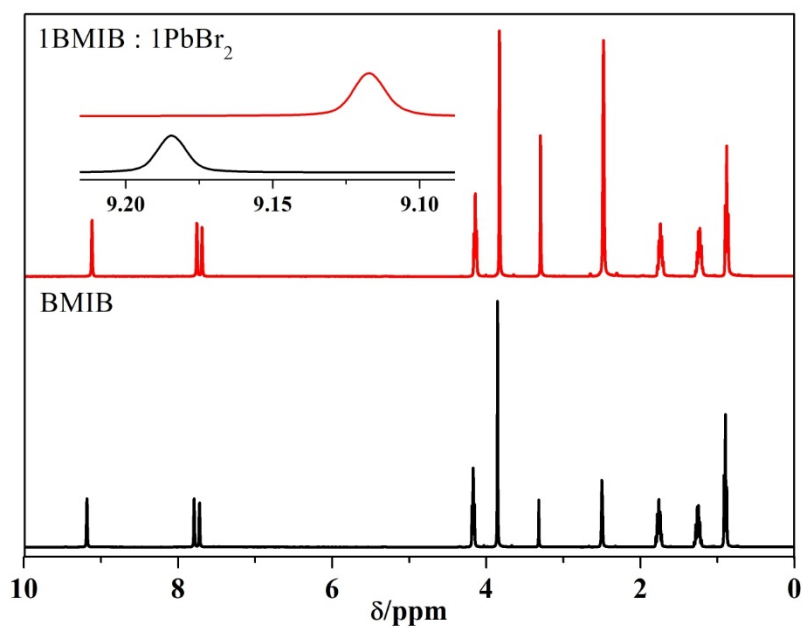


Figure S7. ^1H NMR spectrum of BMIB and mixture of BMIB : PbBr₂ (1:1) in DMSO-d₆ solution.

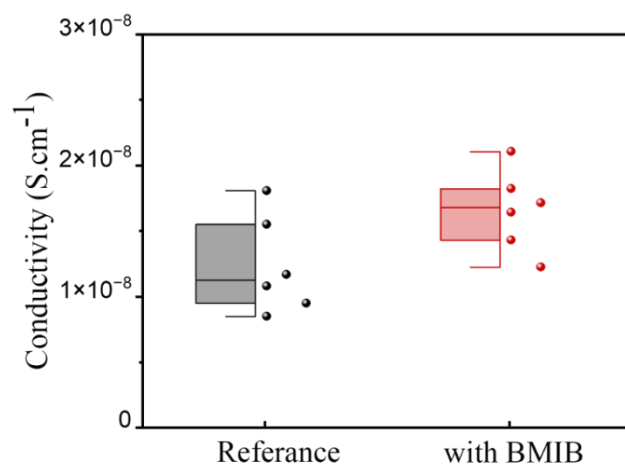


Figure S8. Conductivity of the reference and BMIB-based MAPbBr₃ SCs.

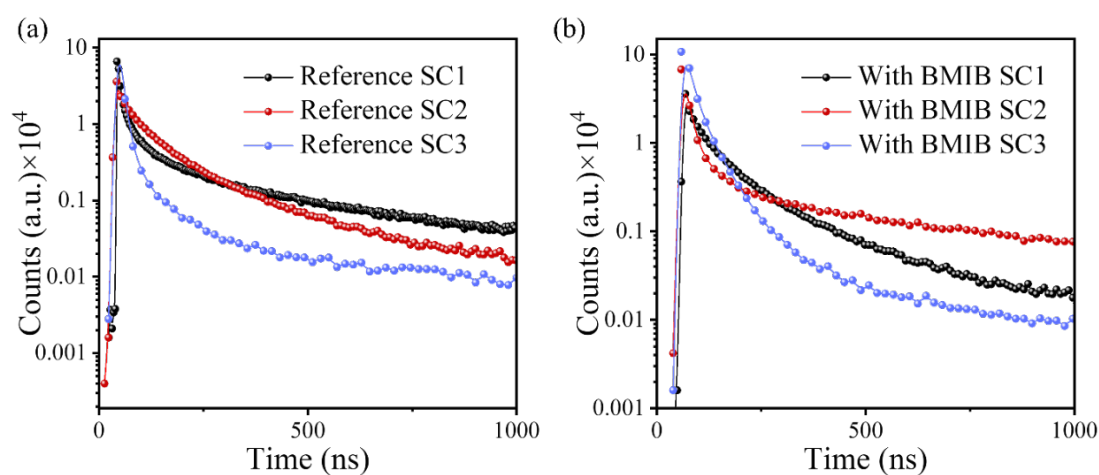


Figure S9. (a) Time-resolved photoluminescence (TRPL) of the three different reference and BMIB-based MAPbBr₃ SCs.

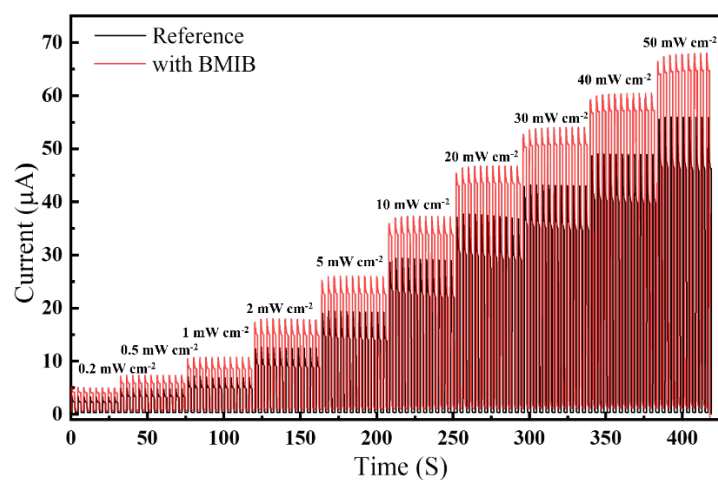


Figure S10. Intensity-dependent transient photoresponse of the reference MAPbBr₃ SC-based PD and BMIB-based PD under light pulse.

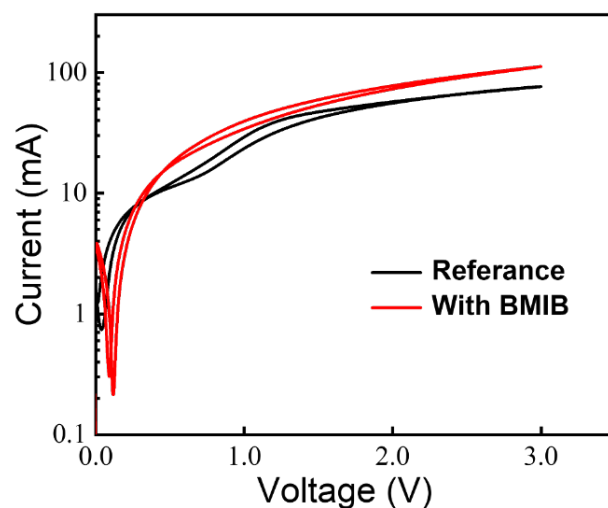


Figure S11. I - V characteristics at 50 W cm^{-2} in forward and reverse scan directions for both the MAPbBr₃ SC-based PD. Scan rate: 100 mV s^{-1} .

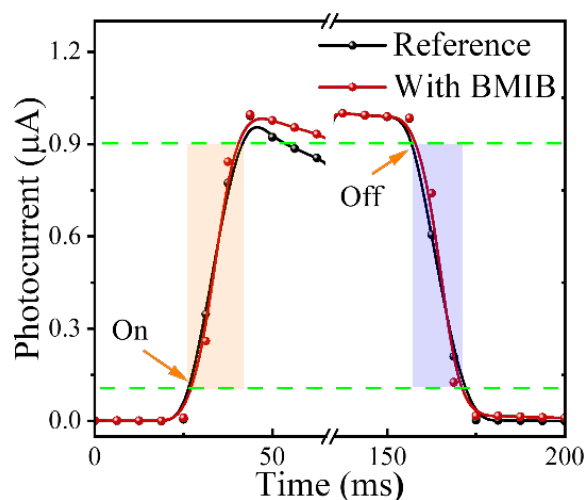


Figure S12. Response speed of the reference and BMIB-based PDs at 1 mW cm^{-2} irradiance power of green light (530 nm) at 2 V.

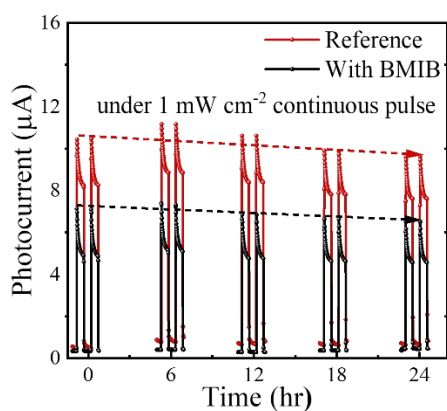


Figure S13. Functional stability of the reference and BMIB-based PDs under 1 mW cm^{-2} irradiance power of green light (530 nm) at 2 V.

Table S1. Comparison of nucleation time and growth time of MAPbBr₃ SCs.

Methods	Temperature	Nucleation time	SCs / growth time
without (reference)	60 °C	N/A	NA / 12 h
	80 °C	30 min	Large SCs / 4h
with BMIB 1 mol%	60 °C	5 h	Small SCs / 24 h
with BMIB 3 mol%	60 °C	4 h	Small SCs / 24 h
with BMIB 5 mol%	60 °C	90 min	Large SCs / 12h
with BMIB 10 mol%	60 °C	N/A	NA / 12 h

Table S2. Average growth rate of MAPbBr₃ SCs.

Methods	Temperature	Nucleation time	Collected SCs weight after 6h growth time	Average growth rate
without (reference)	80 °C	30 min	397	1.1 mg / min
with BMIB 5%		60 min	286 mg	0.8 mg / min

Table S3. Calculated lattice strain of reference and (b) BMIB-based MAPbBr₃ SCs.

peak position 2θ (deg)	FWHM (deg)		lattice strain (%)	
	without (reference)	with BMIB 5 mol%	without (reference)	with BMIB 5 mol%
14.98	0.30	0.19	0.996	0.631
30.22	0.29	0.23	0.469	0.372
45.99	0.41	0.24	0.422	0.247

Table S4. The comparison of the performance parameters for pure MAPbBr₃ SC based PDs growth by ITC and our work.

Device	Growth temp. (°C)	Seeded /Additive	Duration	Wavelength (nm) / Bias (V)	R (AW ⁻¹)	D* Jones	EQE (%) /Gain	On/off time	Ref
Pt/MAPbBr ₃ /Pt	80	-	4h	448 nm 2 V	1.99	5.09 × 10 ¹²	553		1
Cr/MAPbBr ₃ /Au	60	-	20 days	515 nm 5 V	55.7	8 × 10 ¹³	13453	120 ms / 86 ms	2
Pt/MAPbBr ₃ /Pt	110	-	-	White light 2V	0.059	-	-	<20 ns / 500 μs	3

Au/MAPbBr ₃ /Au	80	-	-	350 nm	-	-	900	-/ 30 μs	4
Au/MAPbBr ₃ /Au	85	seeded	-	405 nm 9.84 V	0.038 (110)	-	0.113 (110)	0.153 s / 0.057 s	5
Au/MAPbBr ₃ /Au	80	-	-	576 nm 2 V	5.3	7.4 × 10 ¹¹	1130	3.90 ms / 4.09 ms	6
C/MAPbBr ₃ / C	65	Seeded	6 h	473 nm 5 V	5.49	5.35 × 10 ¹¹			7
Pt/MAPbBr ₃ / Pt	80	-	4 h	530 nm 2V	3.5	7.8 × 10 ¹²	839	14.3 ms / 16.1 ms	This wor k
	60	BMIB IL	12 h	530 nm 2V	4.81	9.35 × 10 ¹²	1124	12.1 ms / 14.8 ms	

Supplementary Note 1. The lattice strain from XRD was calculated by using the HighScore analysis software from PANanalytical. The lattice strain (%) is calculated by the tangent formula:

$$lattice\ strain = \frac{B_{struct}}{4 \tan \theta} \quad (S1)$$

where, B_{struct} describes the structural broadening by:

$$B_{struct} = \sqrt{B_{obs}^2 - B_{std}^2} \quad (S2)$$

where, B_{obs} and B_{std} are breadth obtained from the sample to be analyzed and breadth obtained from the standard sample, respectively.⁸

Supplementary Note 2.

Responsivity (R), Specific Detectivity (D*) and External Quantum Efficiency (EQE) are important parameters for a PD. The photoresponse (R) of the PD, was calculated using the formula:¹

$$R = (J_{ph} - J_d)/P \quad (S3)$$

where the J_{ph} is the photocurrent density, J_d is the dark current density, and P is the illumination power. The D^* of the PD, was calculated by the equation; ¹

$$D^* = R/\sqrt{(2qJ_d)} \quad (S4)$$

where, q is the charge of electron.

The EQE of the PDs were calculated by; ¹

$$EQE = Rhc/e\lambda \quad (S5)$$

The Rise time are calculated from time taken to reach 10% to 90% of the photocurrent value after switch on light and fall-time are calculated from time taken to decay 90% to 10% of the photocurrent value after switch off light of a PDs (extracted from the normalized photocurrents).⁹

References

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