Supporting Information

Cl-doped $FAPbBr_3$ single crystals with stabilized lattice and suppressed surface vacancies for environmentally stable photodetectors

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Notes

The authors declare no competing financial interest.

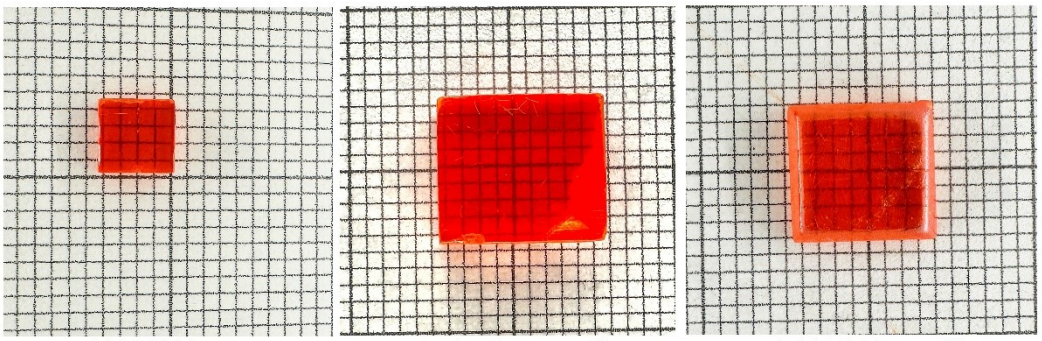

Figure S1. Photos of as-grown $FAPbBr_3$ SC and $FAPbBr_{3-x}Cl_x$ SC with Cl/(Cl+Br) ratios varying from 0% to 6.6%.

The ratio of Cl and Br elements in a mixed halide perovskite can indeed be estimated using Vegard's law, which relates the lattice parameter of the solid solution to the composition of its components. For the (001) plane Vegard's law can be described as:

$$sin\theta = \frac{\lambda}{2(xa_{FAPbCl_3} + (1-x)a_{FAPbBr_3})}$$

Where: θ is the Bragg angle, λ is the X-ray wavelength, d is the interplanar spacing. a_{FAPbCl_3} and a_{FAPbBr_3} are the lattice parameters of pure FAPbCl3 and FAPbBr3. Calculated lattice parameters of a_{FAPbCl_3} and a_{FAPbBr_3} are 5.738 Å and 5.997 Å.

Table S1. Calculated Cl molar ratio of the FAPbBr3-xClx SCs.

SC	$FAPbBr_3$	$FAPbBr_{2.9}Cl_{0.1}$	$FAPbBr_{2.8}Cl_{0.2}$	$FAPbBr_{2.7}Cl_{0.3}$	$FAPbBr_{2.6}Cl_{0.4}$
θ	14.76	14.78	14.81	14.82	**14.85**
Cl/ Br + Cl	0	3.1%	7.5%	9.2%	**13.84%**

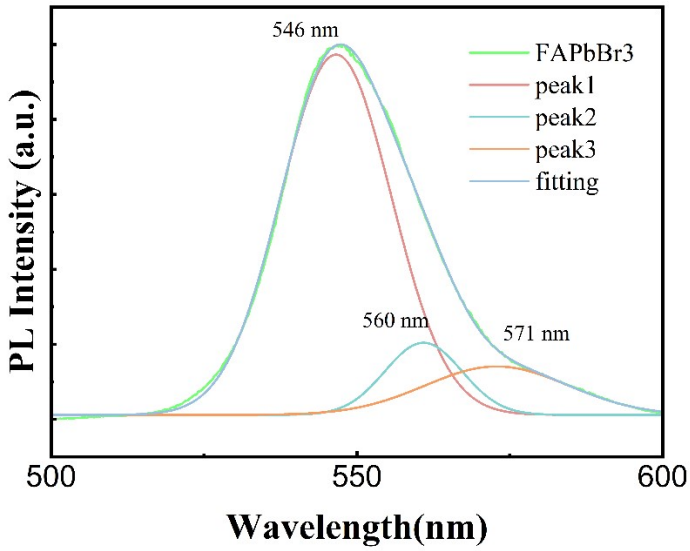

Figure S2. PL spectra of $FAPbBr_3$ SC after stored in ambient air for three months.

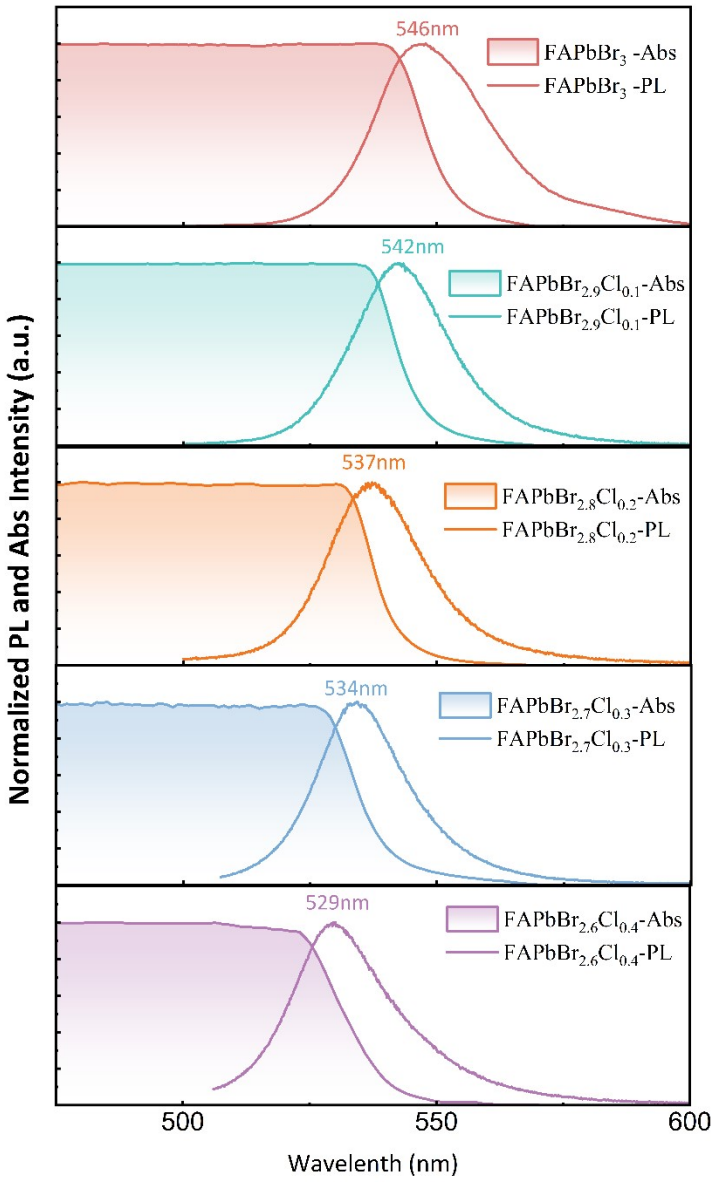

Figure S3. PL and absorption spectra of the $FAPbBr_{3-x}Cl_x$ (x=0, 0.1, 0.2, 0.3 and 0.4) samples.

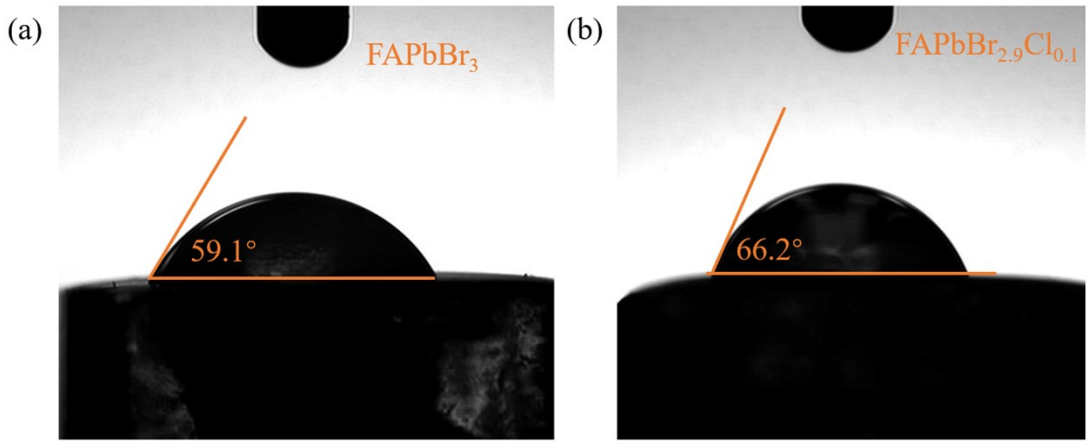

Figure S4. Water contact angle of the $FAPbBr_{3-x}Cl_x$ (x=0 and 0.1) samples.

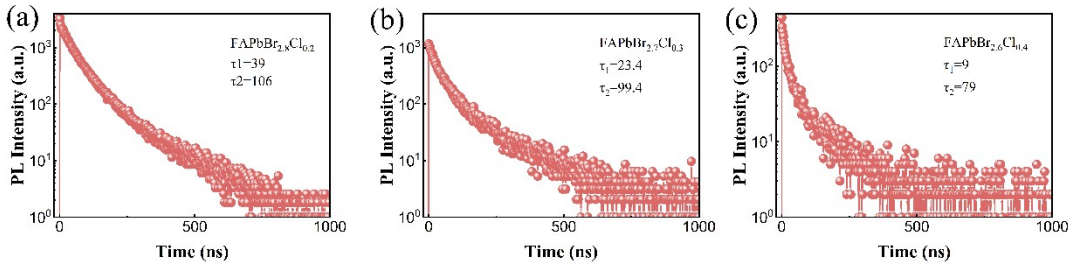

Figure S5. Carrier recombination lifetimes of $FAPbBr_{3-x}Cl_x$ (x=0.2, 0.3 and 0.4) SCs measured by time-resolved photoluminescence (TRPL).

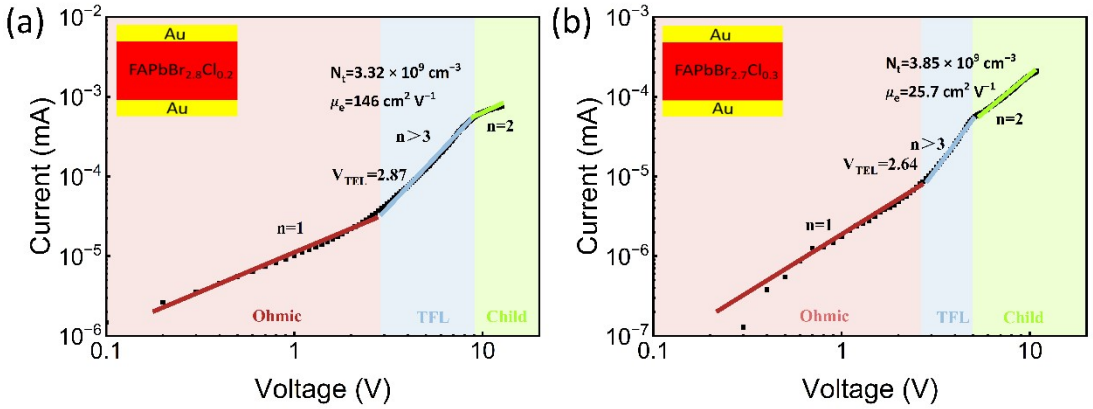

Figure S6. Current–voltage curve for electron-only devices of $FAPbBr_{3-x}Cl_x$ (x=0.2 and 0.3) SCs.

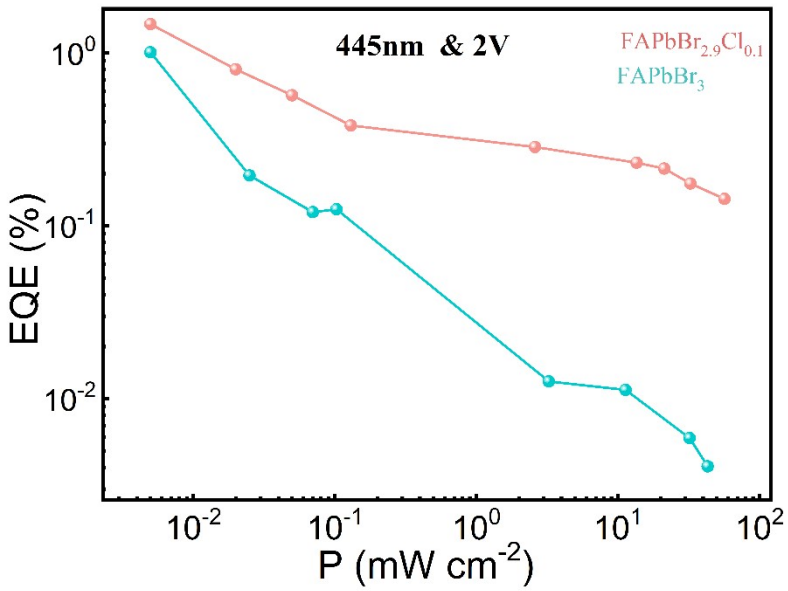

Figure S7. EQE under different Light intensity.

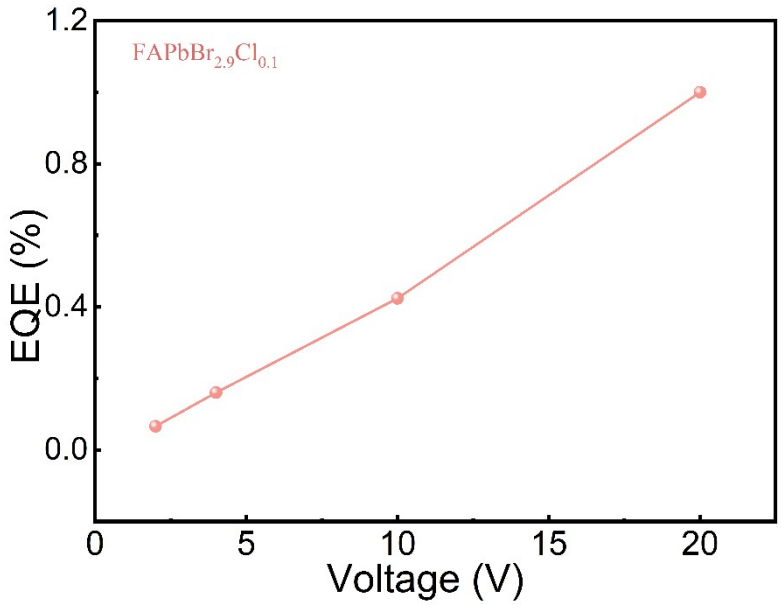

Figure S8. EQE under different voltage

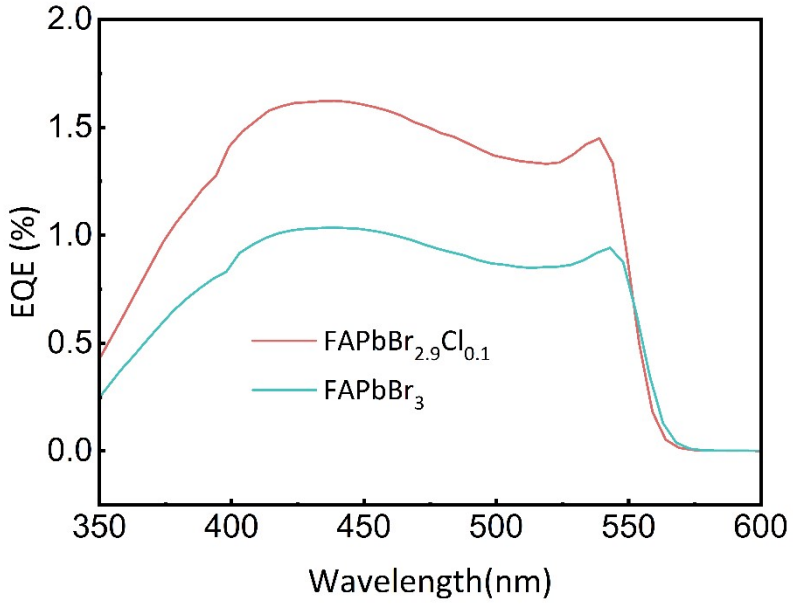

Figure S9. EQE of $FAPbBr_3$ SC and $FAPbBr_{2.9}Cl_{0.1}$ device.

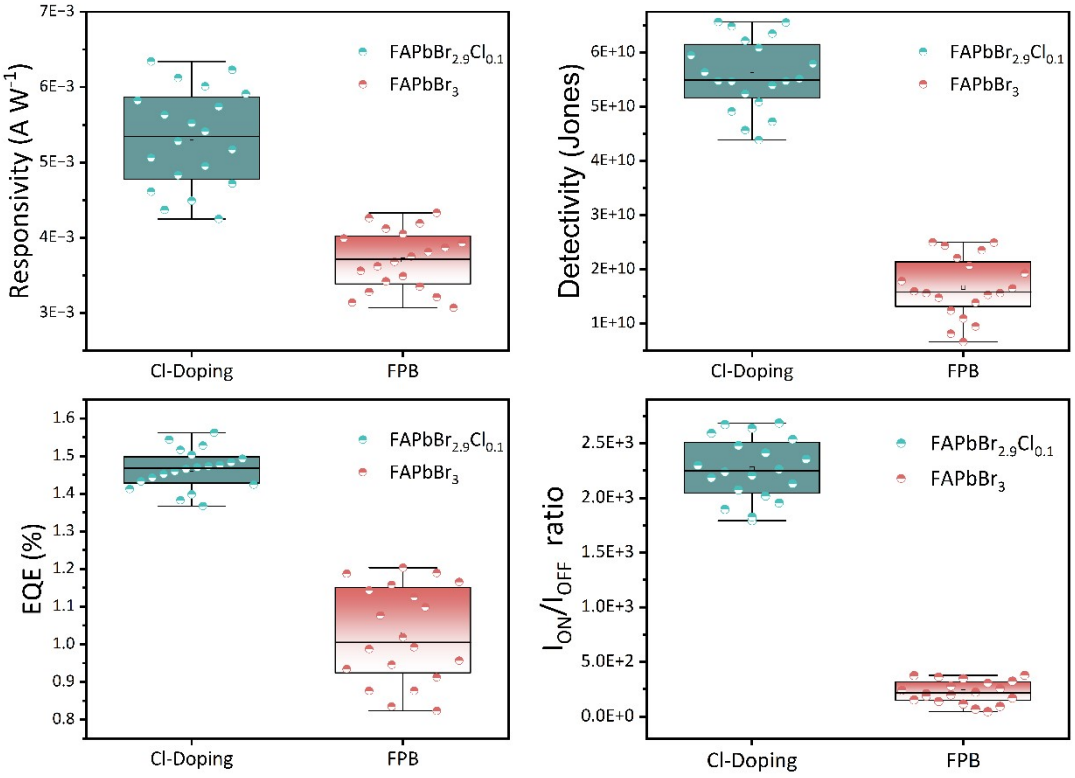

Figure S9. Error analysis of $FAPbBr_3$ SC and $FAPbBr_{2.9}Cl_{0.1}$ device parameters.

Table S2. Comparison of the key performance parameter for perovskite single crystal photodetectors reported in literature and our work.

Materials	Bias/ Light Intensity	R (mA W^{-1})	EQE (%)	Detectivity (Jones)	Refs.
$MAPbBr_3$	9.84 V/ 10 μ W	15	0.046		[1]
$MAPbCl_3$	15 V/	46.9		1.2×10^{10}	[2]
$MAPbBr_3/MAPbI_3$	0.7 V/ 0.01W	0.046		1.75×10^{10}	[3]
$MAPbI_3$	0 V/ 0.01mW	1.5		3.4×10^{7}	[4]
$FAPbBr_{2.5}I_{0.5}$	0 V/0.647 mW	59.89	34.51	4.95×10^{10}	[5]
$FAPbBr_3$	0 V/ 1 m W	0.18	0.055	1.6×10^{8}	[6]
$FAPbBr_3$	2V 5 μ W	5.3	1.46775	5.47×10^{10}	**This work**

References

1 Z. Zuo, J. Ding, Y. Zhao, S. Du, Y. Li, X. Zhan and H. Cui, *J. Phys. Chem. Lett.*, 2017, **8**, 684–689.

2 G. Maculan, A. D. Sheikh, A. L. Abdelhady, M. I. Saidaminov, M. A. Haque, B. Murali, E. Alarousu, O. F. Mohammed, T. Wu and O. M. Bakr, *J. Phys. Chem. Lett.*, 2015, **6**, 3781–3786.

3 B. Huang, J. Liu, Z. Han, Y. Gu, D. Yu, X. Xu and Y. Zou, *ACS Appl. Mater. Interfaces*, 2020, **12**, 48765–48772.

4 Z. Yang, H. Wang, L. Guo, Q. Zhou, Y. Gu, F. Li, S. Qiao, C. Pan and S. Wang, DOI:10.1002/smll.202101572.

5 F.-X. Liang, L.-L. Zhou, Y. Hu, S.-F. Li, Z.-Y. Zhang, J.-Y. Li, C. Fu, C.-Y. Wu, L. Wang, J.-A. Huang and L.-B. Luo, *Adv. Funct. Mater.*, 2023, **33**, 2302175.

6 S.-T. Dong, Z. Fu, M. Yu, J.-L. Jiang, X. Jin, Y.-H. Guo, L. Wang and Y.-M. Zhang, *CrystEngComm*, 2022, **24**, 2100–2106.