Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
This journal is © The Royal Society of Chemistry 2024

Supporting Information

Single- and two-photon excited photoluminescence of 2D perovskite thin films with different organic spacer cations

Tai Luo,[a] Junzi Li,[a] Yanyan Cui,[a] Hao Jin,*[b] and Tingchao He*[a]

[a]Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China. Email: tche@szu.edu.cn

[b]College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China. Email: hjin@szu.edu.cn

The crystallographic structures of $(EA)_2PbBr_4$, $(PA)_2PbBr_4$, and $(BA)_2PbBr_4$ were obtained from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. CCDC numbers 1855044, 2171431 and 1521054 correspond to $(EA)_2PbBr_4$, $(PA)_2PbBr_4$, and $(BA)_2PbBr_4$ films, respectively.

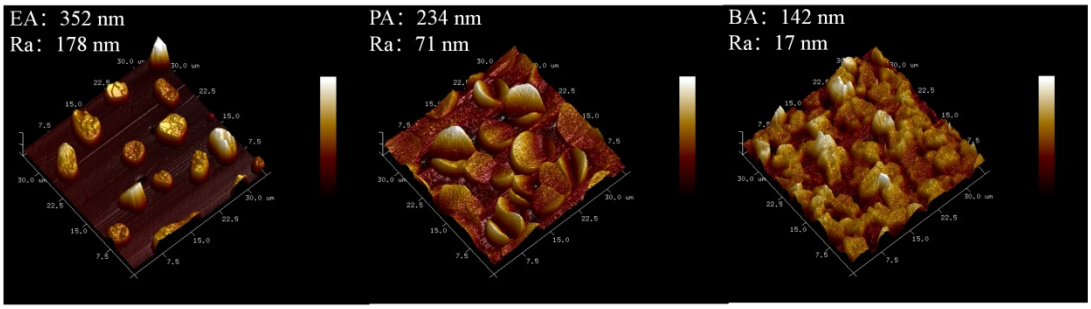

Fig. S1 AFM images of $(EA)_2PbBr_4$, $(PA)_2PbBr_4$, and $(BA)_2PbBr_4$ films.

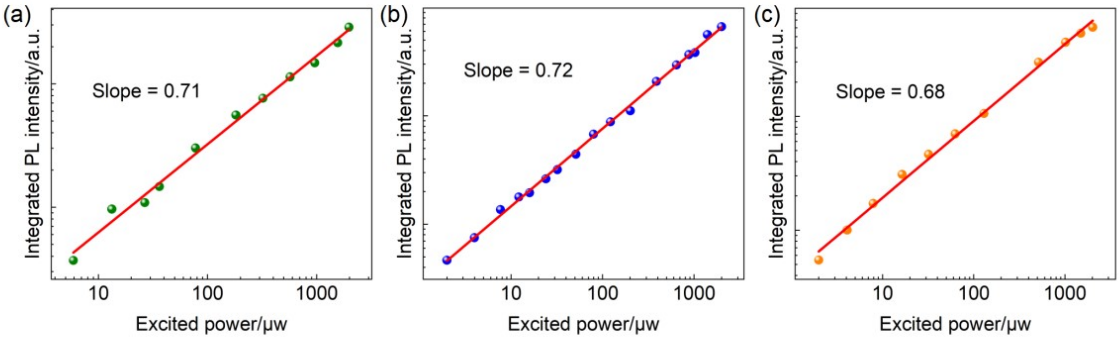

Fig. S2 Integrated PL intensity as a function of excitation power for three samples. (a) $(EA)_2PbBr_4$, (b) $(PA)_2PbBr_4$, and (c) $(BA)_2PbBr_4$ films.

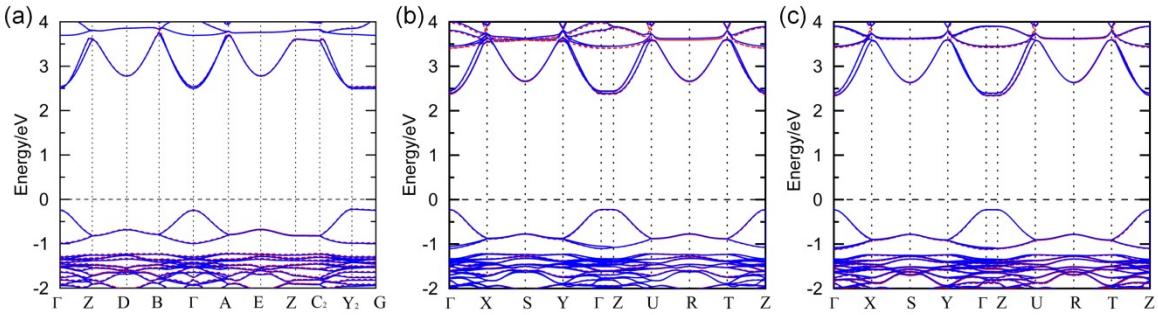

Fig. S3 The calculated band structures for (a) $(EA)_2PbBr_4$, (b) $(PA)_2PbBr_4$ and (c) $(BA)_2PbBr_4$. The red and blue colors represent the results with and without VDW correction.

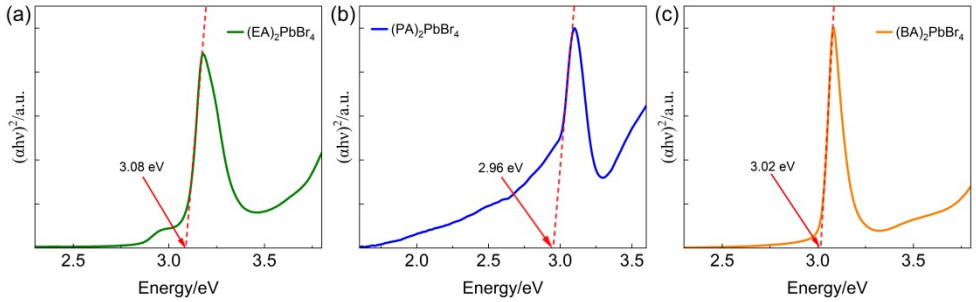

Fig. S4 Tauc plots of (a) $(EA)_2PbBr_4$, (b) $(PA)_2PbBr_4$, and (c) $(BA)_2PbBr_4$ films. The dashed lines represent the corresponding absorption band edges.

Table S1. Band gaps with and without SOC using different functionals.

	with SOC (eV)		without SOC (eV)		Exp. (eV)
	PBE	HSE	PBE	HSE	Tauc
$(EA)_2PbBr_4$	2.01	2.75	2.72	3.50	3.08
$(PA)_2PbBr_4$	1.87	2.58	2.60	3.35	2.96
$(BA)_2PbBr_4$	1.84	2.53	2.56	3.31	3.02

Table S2. Calculated lattice constants (with vs. without VDW correction).

The unit is Å.

	a	*b*	*c*
$(EA)_2PbBr_4$	11.75 vs. 11.75	8.24 vs. 8.24	7.73 vs. 7.73
$(PA)_2PbBr_4$	8.27 vs. 8.29	8.19 vs. 8.21	25.09 vs. 25.15
$(BA)_2PbBr_4$	8.31 vs. 8.32	8.17 vs. 8.18	27.62 vs. 27.66