

Morphology Engineering toward Highly Emissive Mn²⁺ Doped PEA₂PbBr₄ Perovskite with Their LED Application via Phosphonium Passivation

Yu-Feng Sang^{1,3}, Liang-Jin Xu^{1,2*} and Zhong-Ning Chen^{1,2,3*}

¹State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

²Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou 350108, China

³School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China

*Corresponding authors. Emails: xuliangjin@fjirsm.ac.cn and czn@fjirsm.ac.

Table S1. Energy Level of Mn²⁺ Doped PEA₂PbBr₄ QDs Films

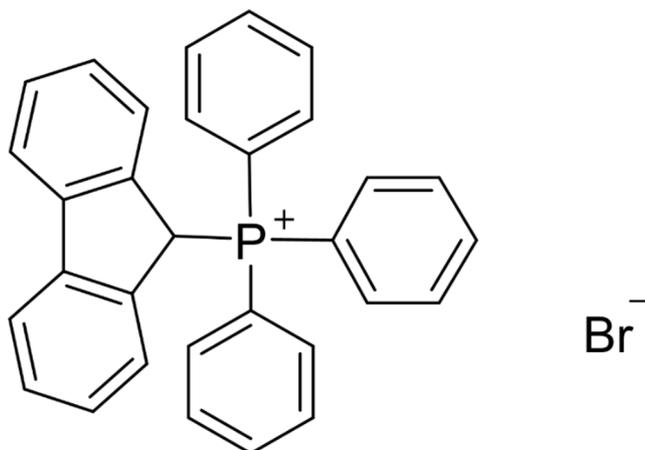
E _{cutoff}	W _F	VBM	CBM
21.22 eV	-5.41 eV	-5.95 eV	-3.59 eV

Table S2. XRF Results of Mn²⁺ Doped PEA₂PbBr₄ QDs Films with Phosphonium Passivated

Element	Ratio (w%)	Element spectrum line	Intensity
Mn	29.3	Mn-KA	0.0794
Pb	70.7	Pb-LA	0.3717

Table S3. FWHM of PXRD Diffraction Peaks

		002	004	006	008	0010	0012	0014
Passivated film	FWHM (angle)	0.28	0.28	0.3	0.42	0.36	0.42	0.3
	FWHM (radian)	0.0049	0.0049	0.0052	0.0073	0.0063	0.0073	0.0052
Pristine film	FWHM (angle)	0.16	0.16	0.18	0.24	0.22	0.22	0.22
	FWHM (radian)	0.0028	0.0028	0.0031	0.0042	0.0038	0.0038	0.0038



Scheme S1. Molecular structure of 9-fluorenyltriphenylphosphonium bromide

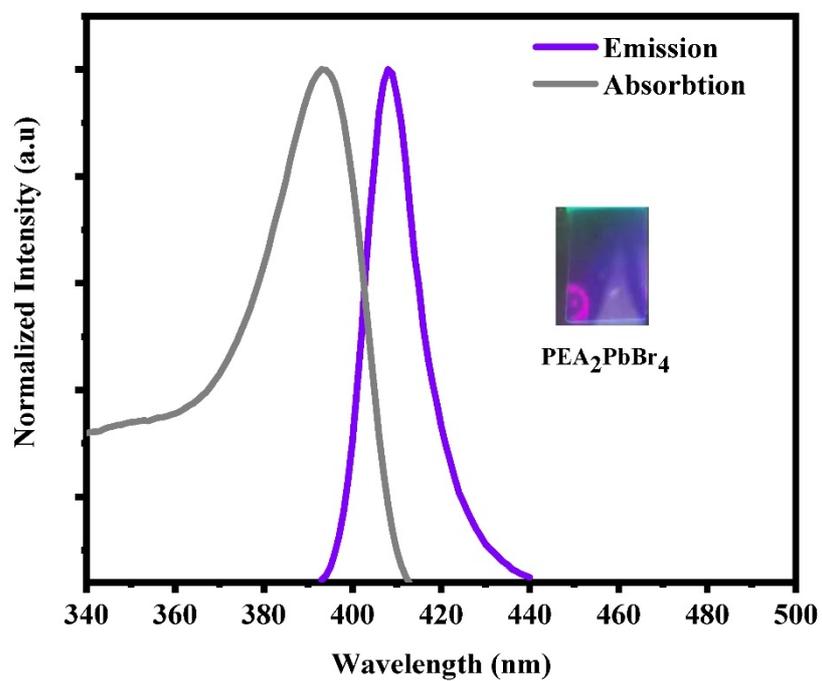


Figure S1. Absorption and emission spectra of PEA₂PbBr₄ films at room temperature.

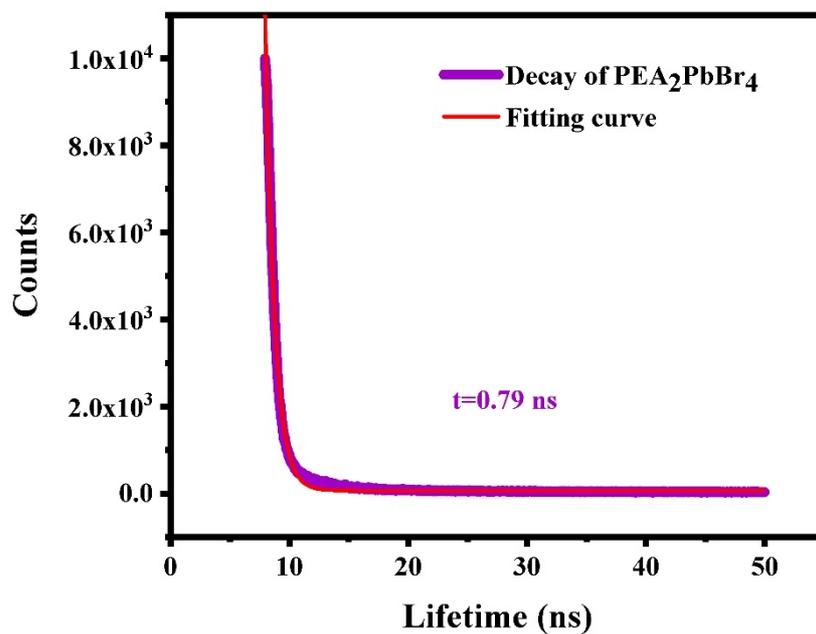


Figure S2. Fluorescence decay and single exponential fitting curve of PEA₂PbBr₄ films at room temperature.

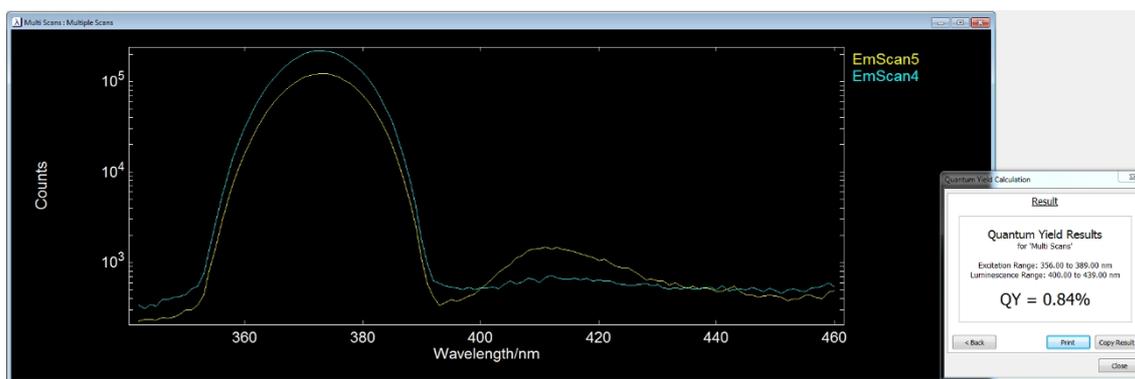


Figure S3. Photoluminescence quantum yield (PLQY) of $\text{PEA}_2\text{PbBr}_4$ films at room temperature.

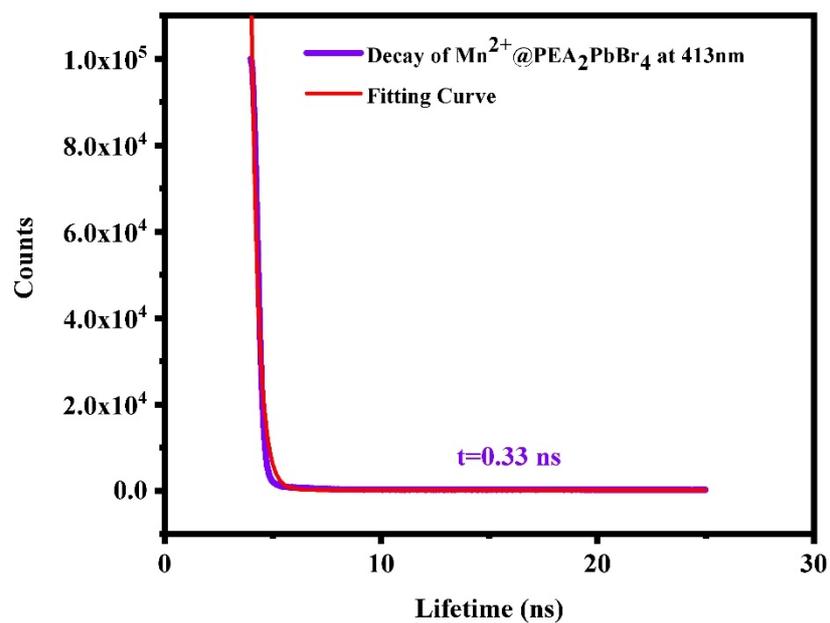


Figure S4. Fluorescence decay and single exponential fitting curve of Mn²⁺ doped PEA₂PbBr₄ films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at 413 nm.

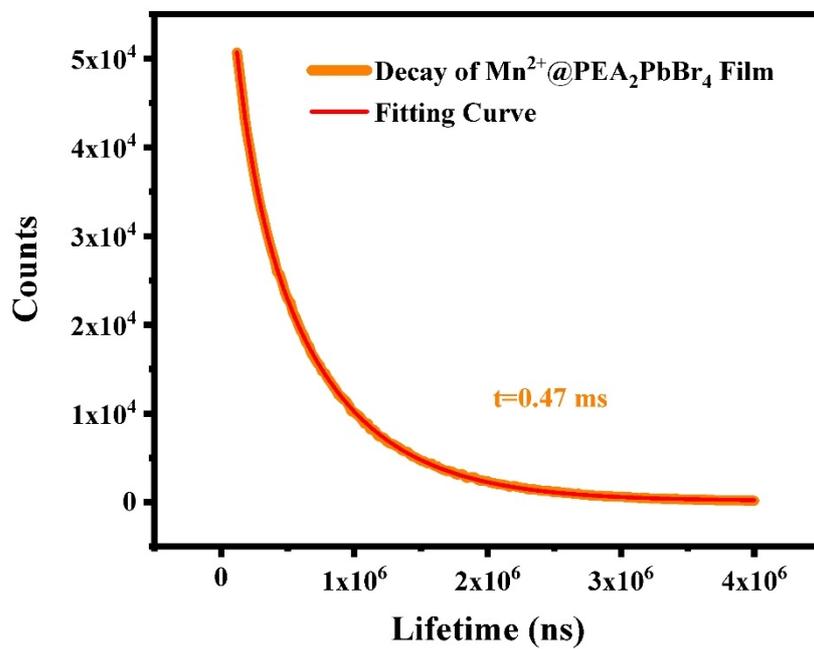


Figure S5. Fluorescence decay and double exponential fitting curve of Mn²⁺ doped PEA₂PbBr₄ films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at 600 nm.

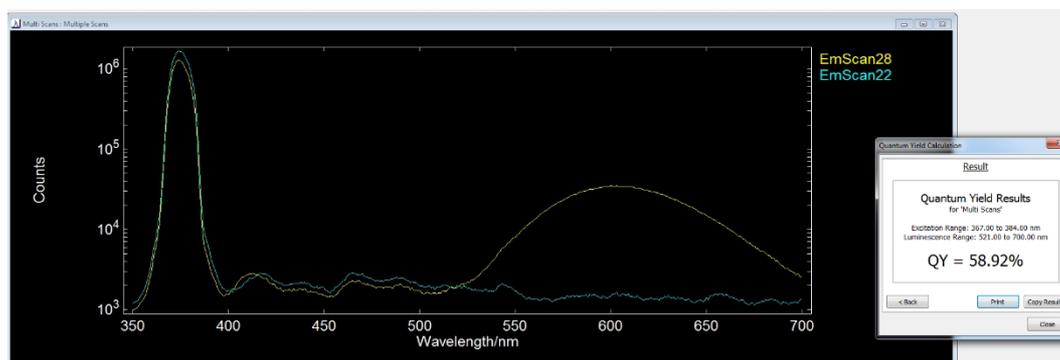


Figure S6. Photoluminescence quantum yield (PLQY) of Mn^{2+} doped $\text{PEA}_2\text{PbBr}_4$ films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at room temperature.

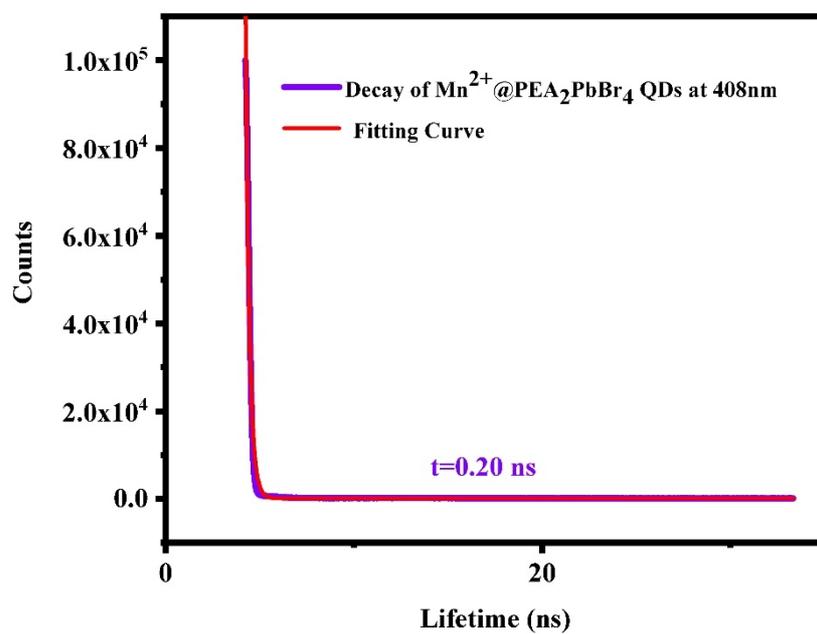


Figure S7. Fluorescence decay and single exponential fitting curve of Mn²⁺ doped PEA₂PbBr₄ in-situ nanocrystals films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at 413 nm.

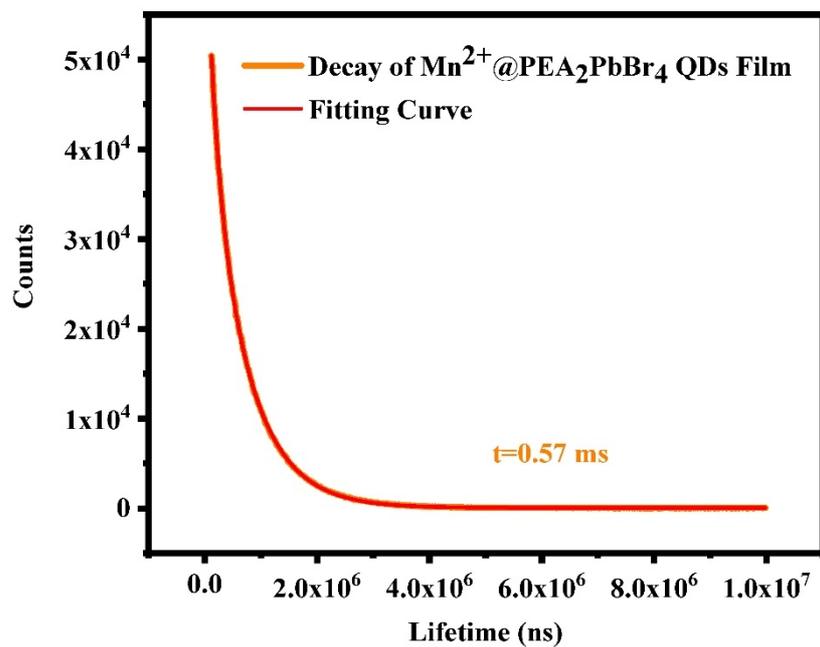


Figure S8. Fluorescence decay and double exponential fitting curve of Mn²⁺ doped PEA₂PbBr₄ in-situ nanocrystals films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at 600 nm.

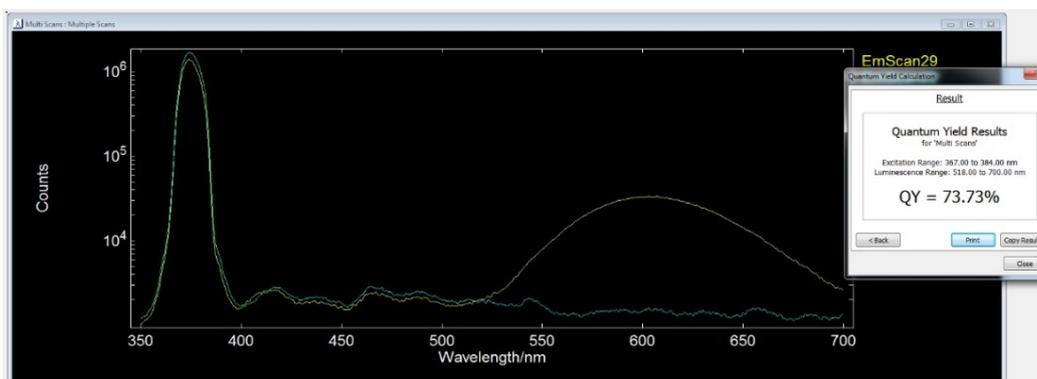


Figure S9. Photoluminescence quantum yield (PLQY) of Mn²⁺ doped PEA₂PbBr₄ QDs films ($V_{\text{Mn}^{2+}}:V_{\text{Pb}^{2+}} = 1:2$) at room temperature.

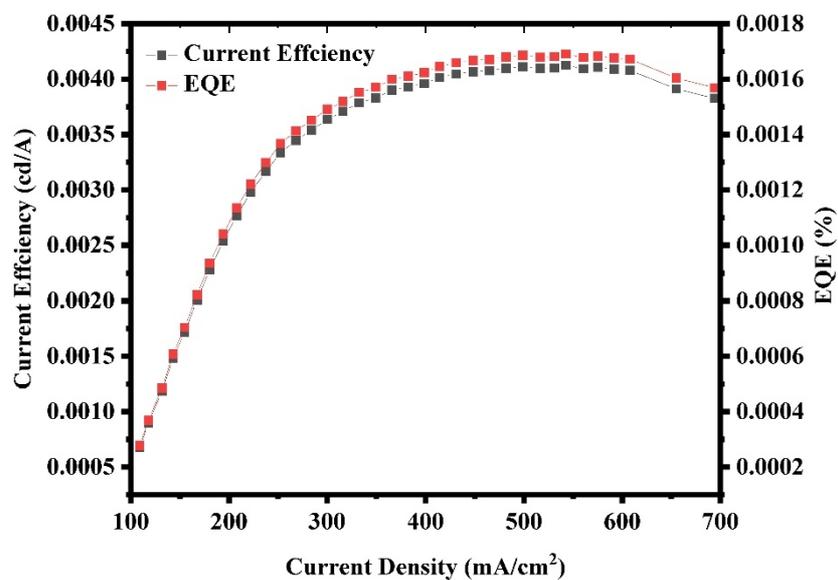


Figure S10. CE-J-EQE curve of LED device based on pristine film.

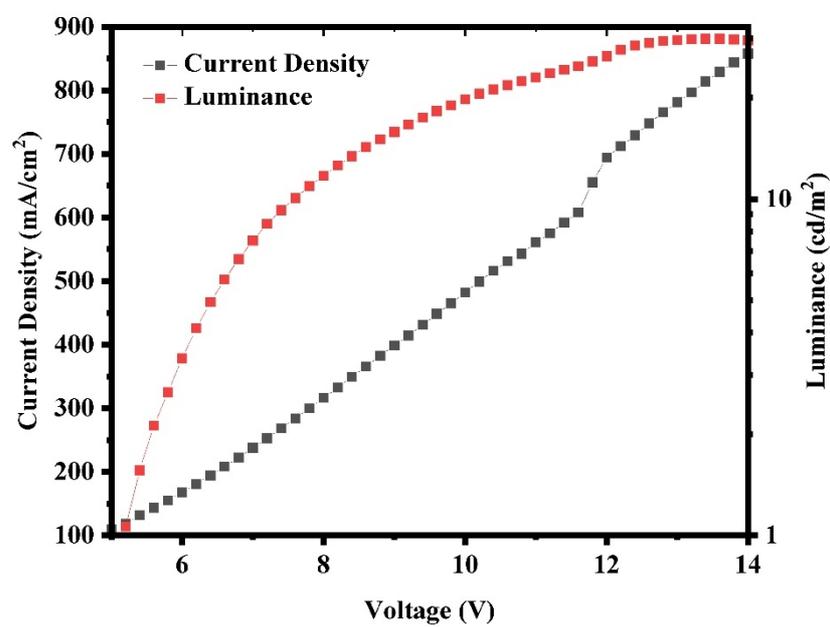


Figure S11. J-V-L curve of LED device based on pristine film.

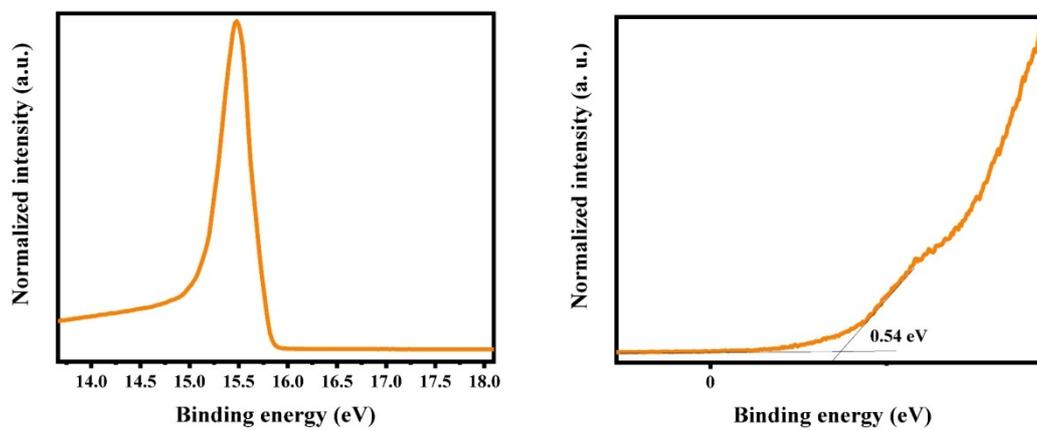


Figure S12. Ultraviolet electron spectroscopy (UPS) of Mn²⁺ doped PEA₂PbBr₄ QDs films.



Figure S13. AFM detection report of pristine film

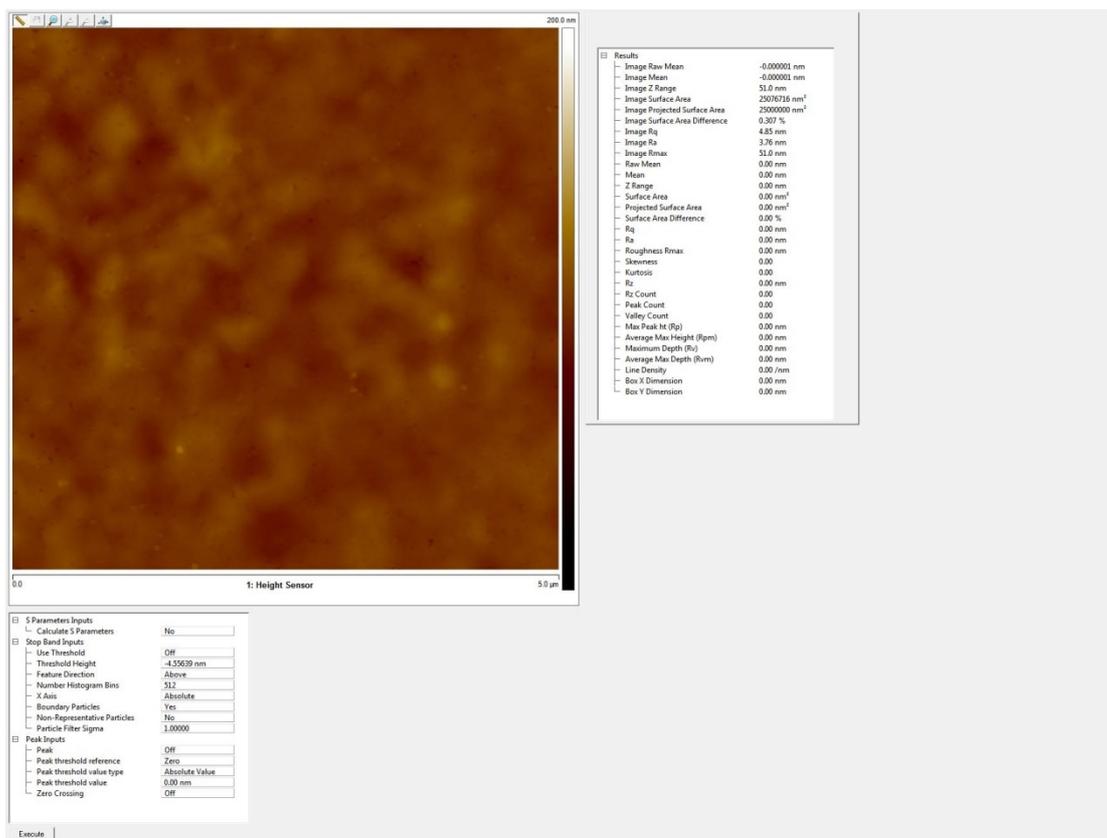


Figure S14. AFM detection report of in-situ passivated film

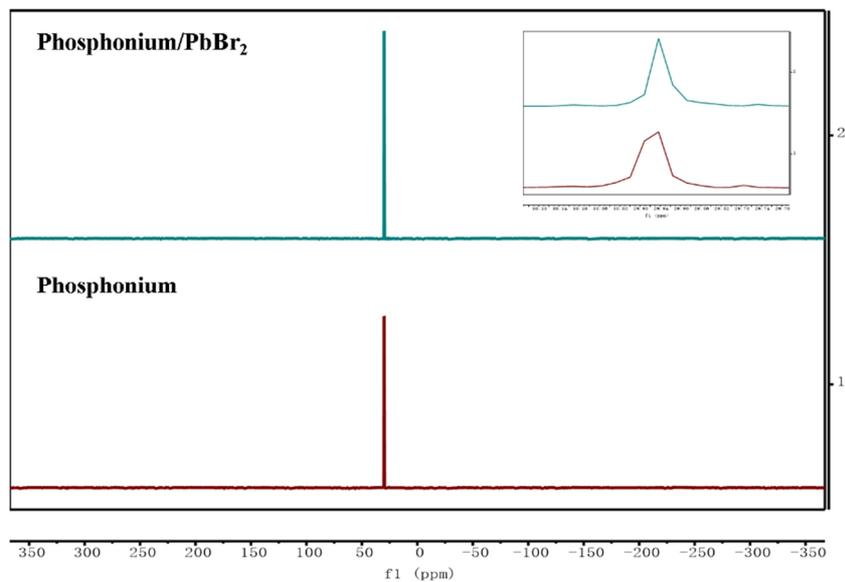


Figure S15. ^{21}P -NMR of phosphonium and phosphonium/ PbBr_2 .

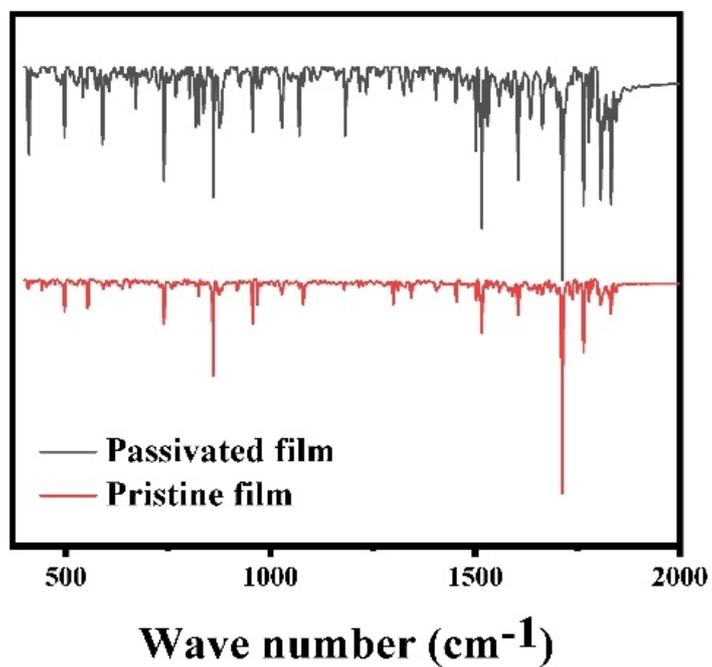


Figure S16. FT-IR of pristine and passivated film.

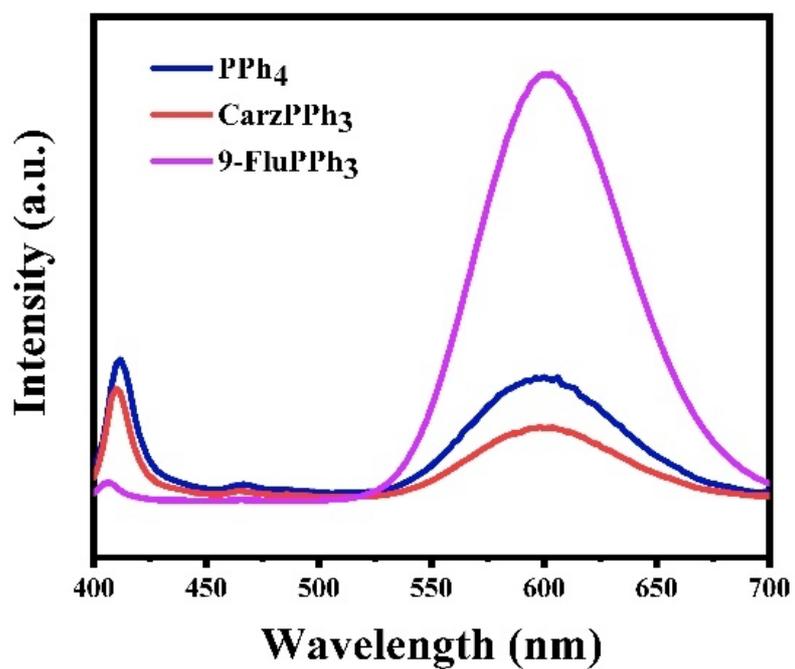


Figure S17. Emission intensity of Mn²⁺ doped PEA₂PbBr₄ films ($V_{\text{Pb}^{2+}}:V_{\text{Mn}^{2+}} = 2:1$) with different phosphonium passivation.

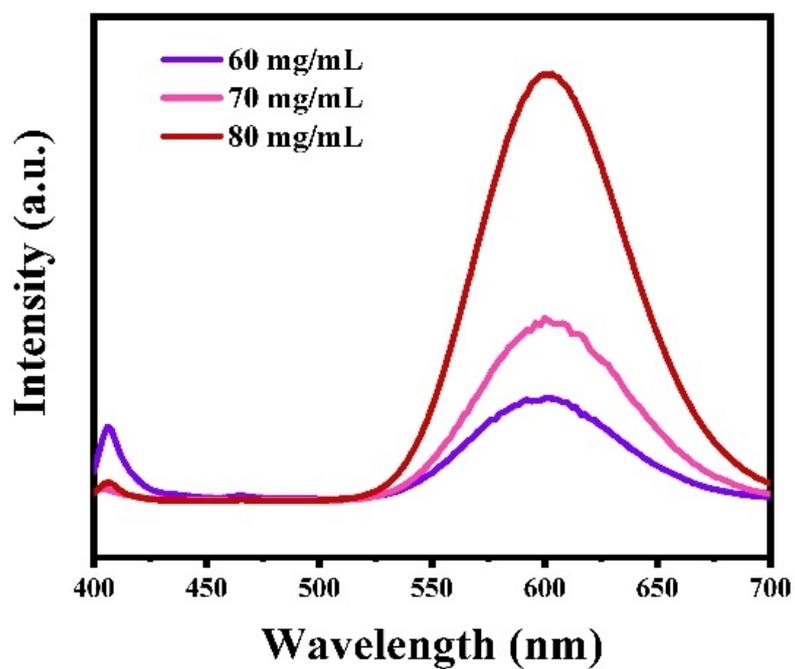


Figure S18. Emission intensity of Mn²⁺ doped PEA₂PbBr₄ films ($V_{\text{Pb}^{2+}}:V_{\text{Mn}^{2+}} = 2:1$) with different amounts of 9-fluorenyl triphenylphosphonium bromide passivation.

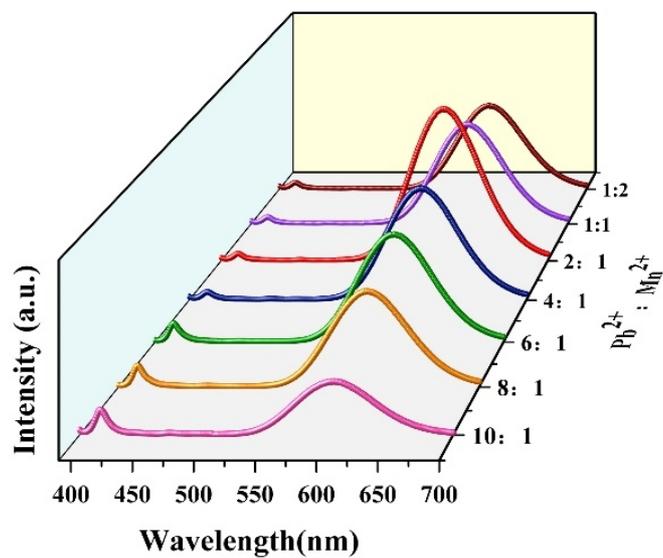


Figure S19. Emission intensity of 9-fluorenyl triphenylphosphonium bromide passivated perovskite quantum wells film with different amounts of Mn²⁺ ratio.