Supporting Information

Enhanced Stability and Tunable Photoluminescence in Mn^{2+}-Doped One-Dimensional Hybrid Lead Halide Perovskites for High-Performance White Light Emitting Diodes

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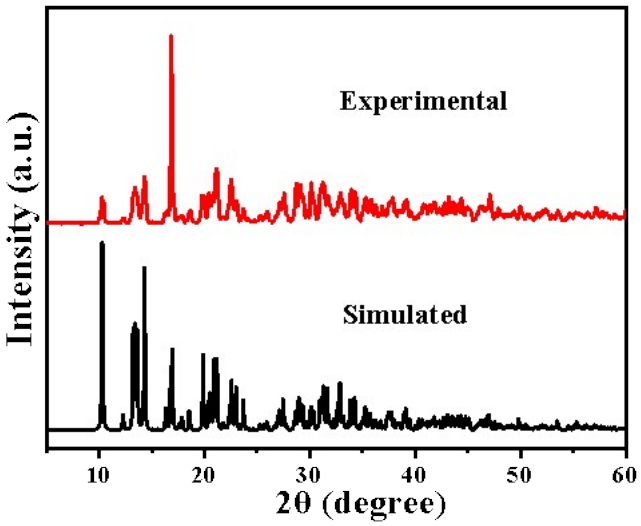


Fig. S1. The simulated and experimental powder X-ray diffraction patterns of compound **1**.

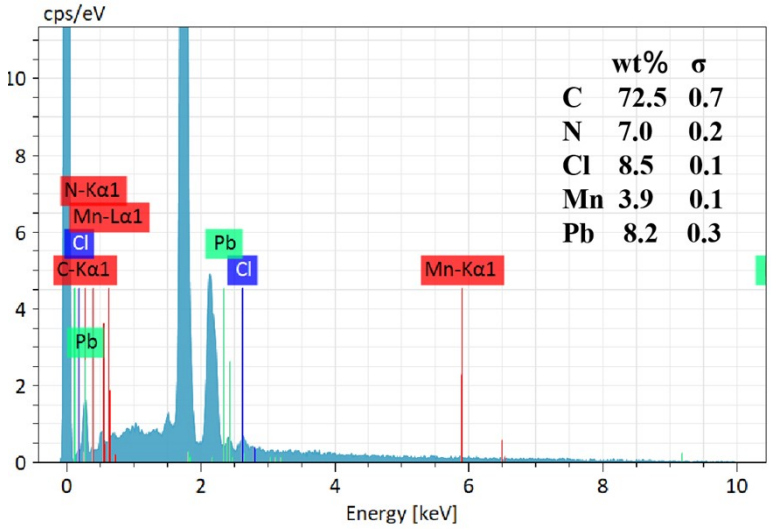


Fig. S2. The EDX analysis result of compound **8**.

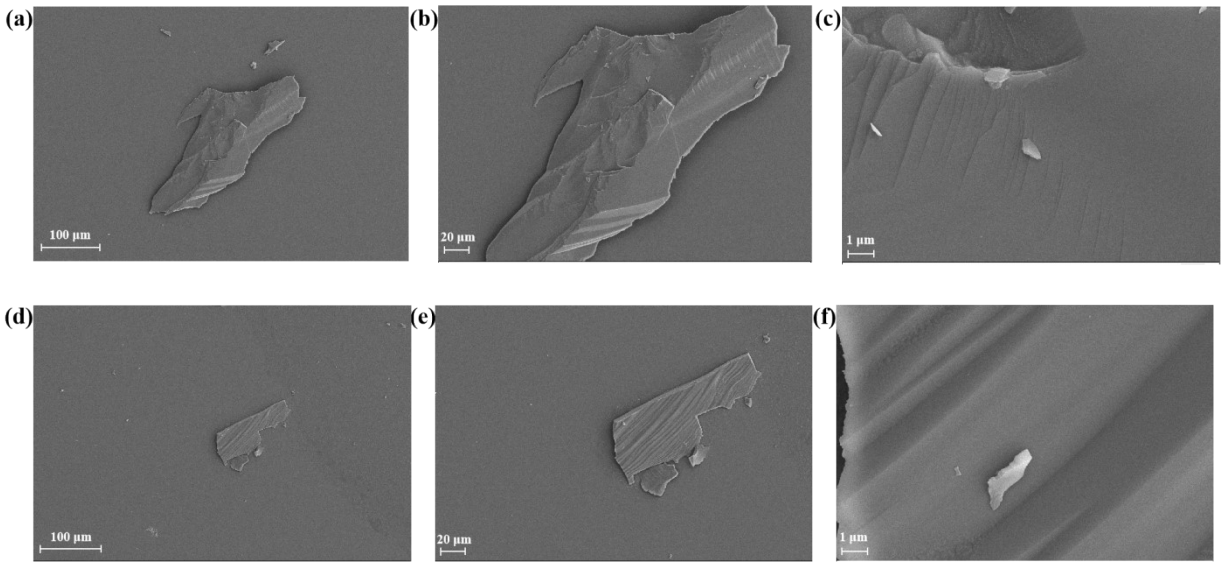


Fig. S3. SEM images compound **1** (a-c) and compound **8** (d-f).

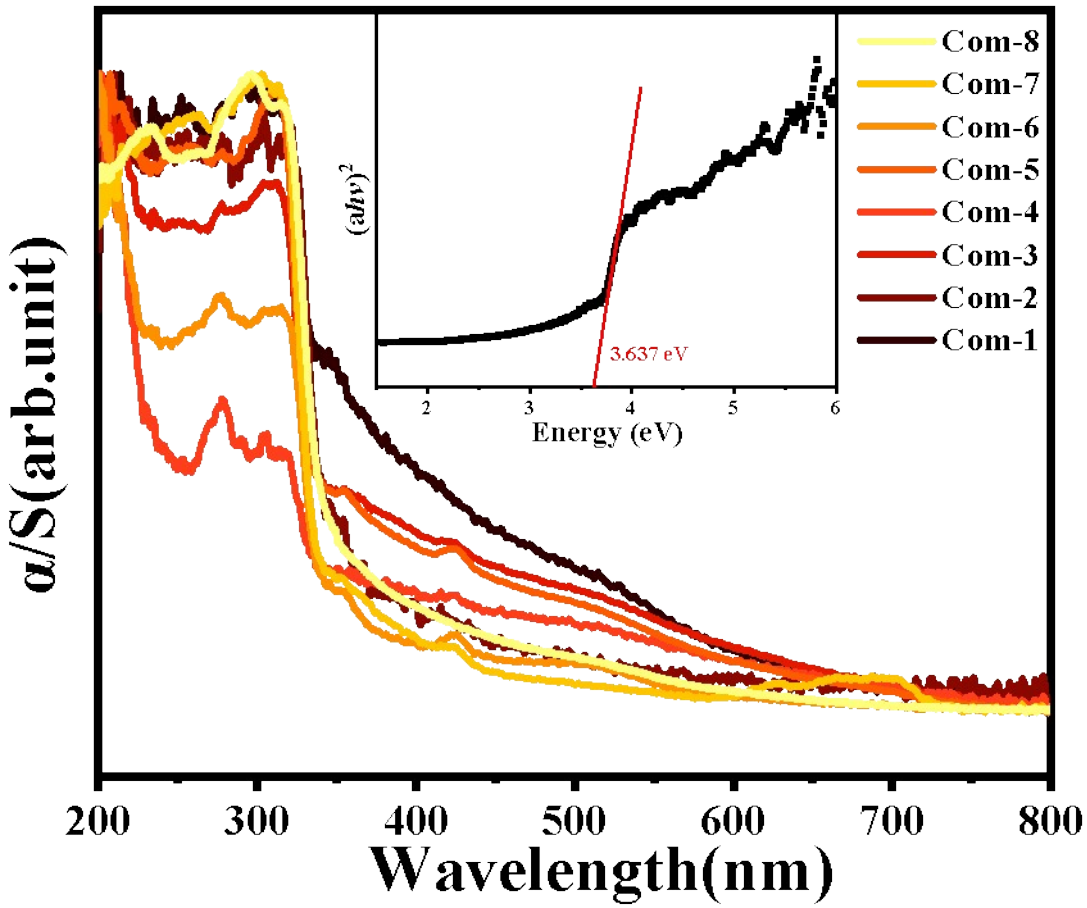
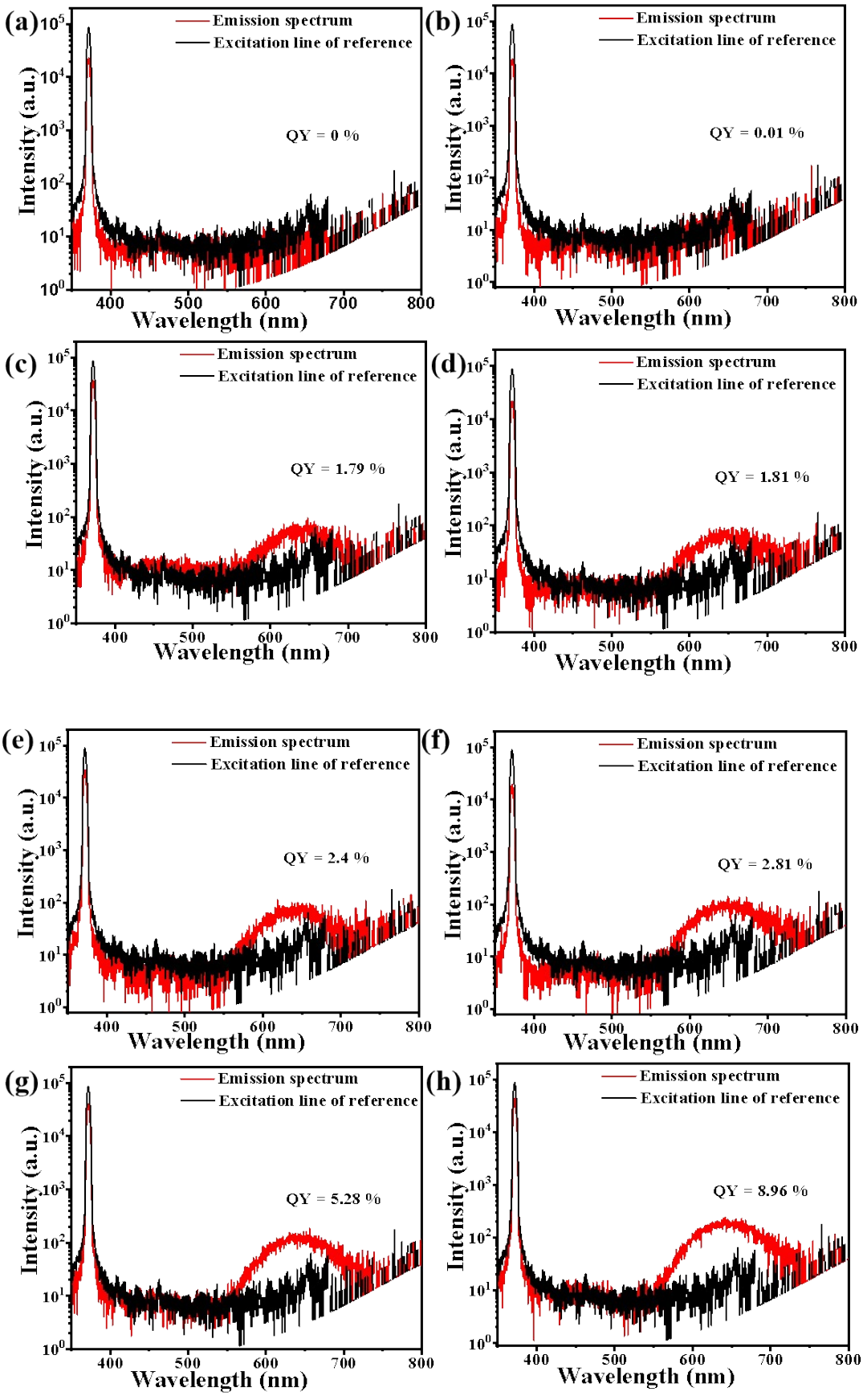


Fig. S4. The solid-state UV-Vis absorption spectra of compounds **1**-**8**.


(a)
Emission spectrum
Excitation line of reference
QY = 0 %
Intensity (a.u.)
Wavelength (nm)
(b)
Emission spectrum
Excitation line of reference
QY = 0.01 %
Intensity (a.u.)
Wavelength (nm)
(c)
Emission spectrum
Excitation line of reference
QY = 1.79 %
Intensity (a.u.)
Wavelength (nm)
(d)
Emission spectrum
Excitation line of reference
QY = 1.81 %
Intensity (a.u.)
Wavelength (nm)
(e)
Emission spectrum
Excitation line of reference
QY = 2.4 %
Intensity (a.u.)
Wavelength (nm)
(f)
Emission spectrum
Excitation line of reference
QY = 2.81 %
Intensity (a.u.)
Wavelength (nm)
(g)
Emission spectrum
Excitation line of reference
QY = 5.28 %
Intensity (a.u.)
Wavelength (nm)
(h)
Emission spectrum
Excitation line of reference
QY = 8.96 %
Intensity (a.u.)
Wavelength (nm)

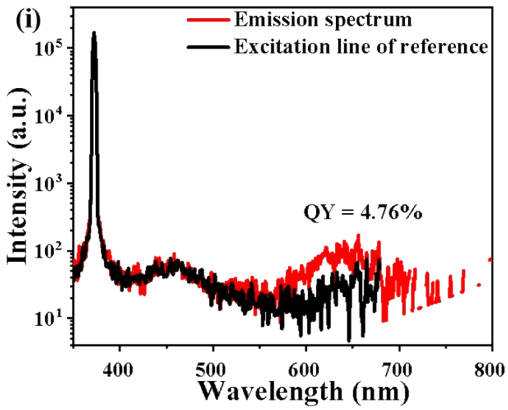


Fig. S5. The PLQYs of compounds **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) , **6** (f), **7** (g), **8** (h), **9** (i).

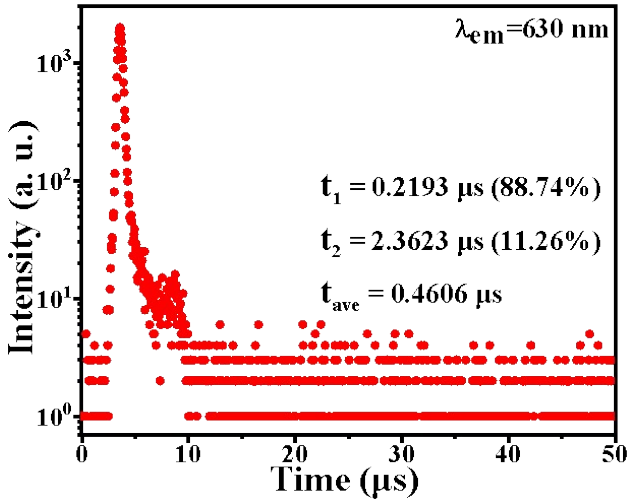


Fig. S6. The PL decay curves monitoring at 630 nm of compound **8** at 300 K.

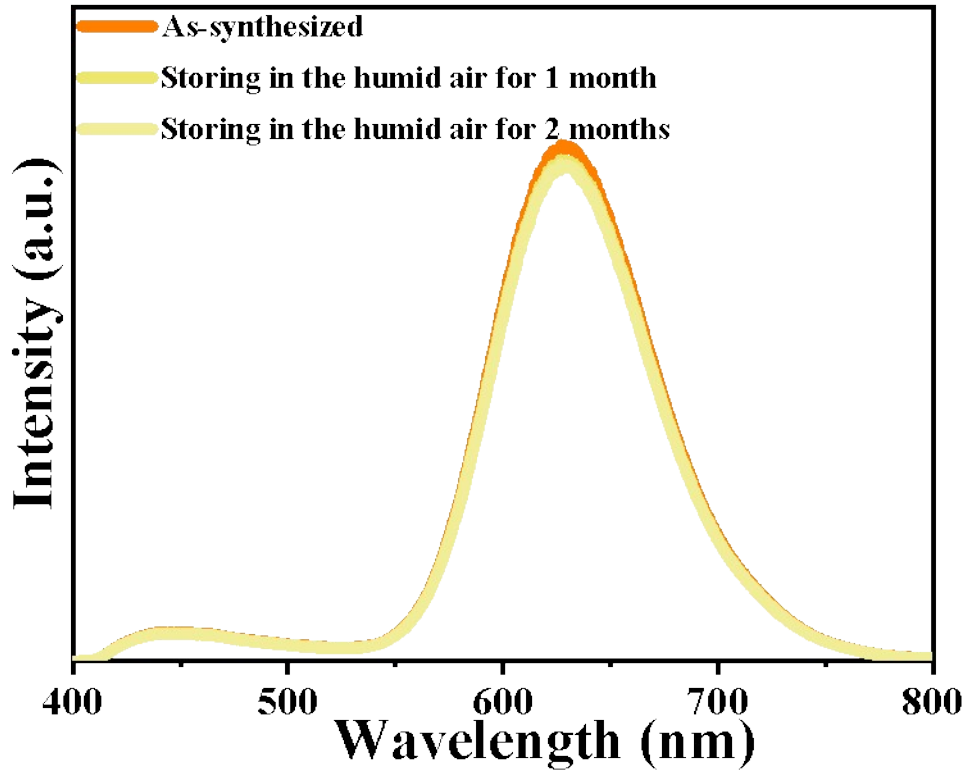


Fig. S7. Comparisons of compound **8** after storing in ambient atmosphere for 1 month and 2 months.

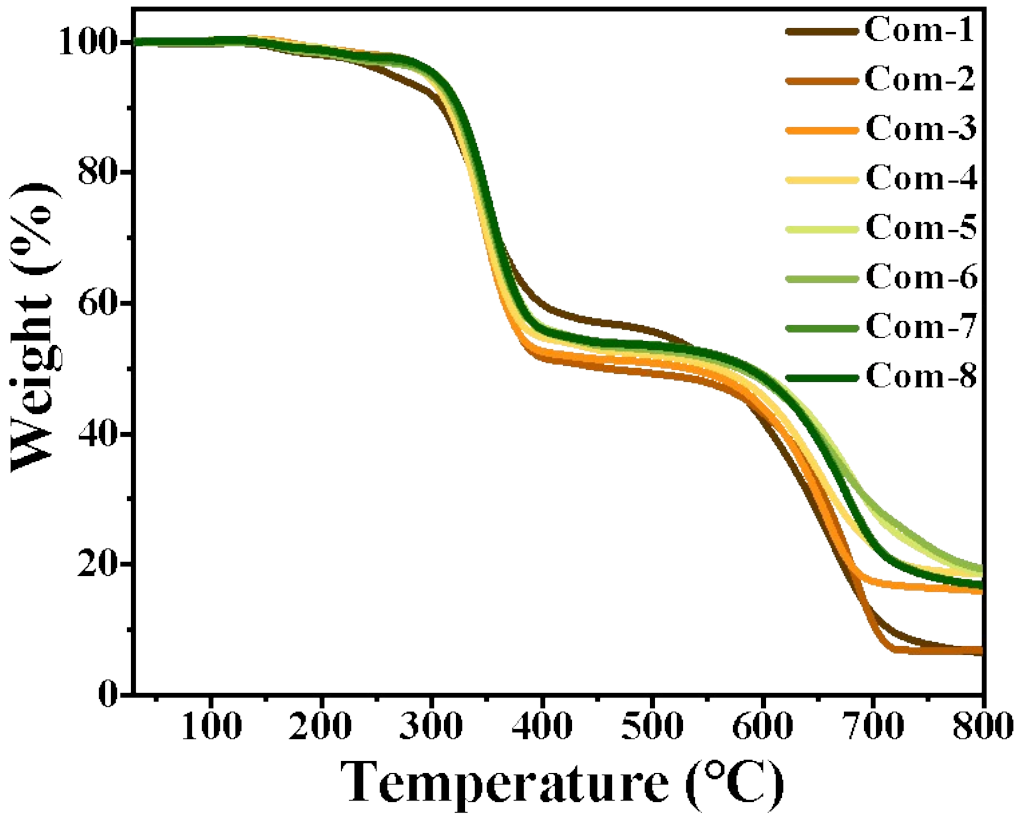


Fig. S8. The thermogravimetric analysis (TGA) curves for selected compounds **1-8**.

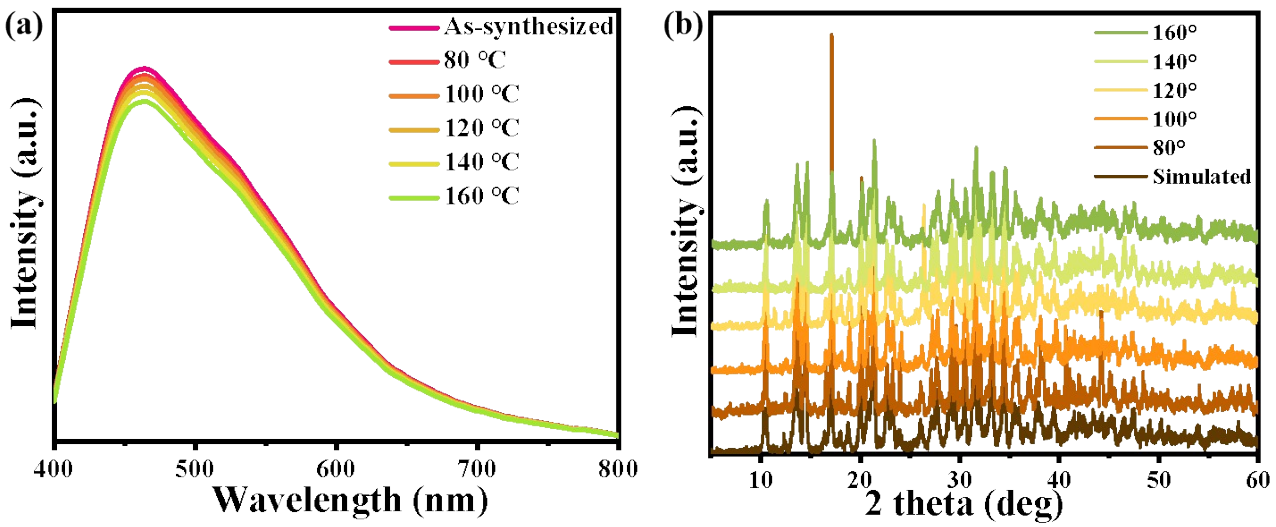


Fig. S9. The pristine and experimental emission spectra (a) and XRD patterns (b) of compound **1** after heating anneal over 10 hours.

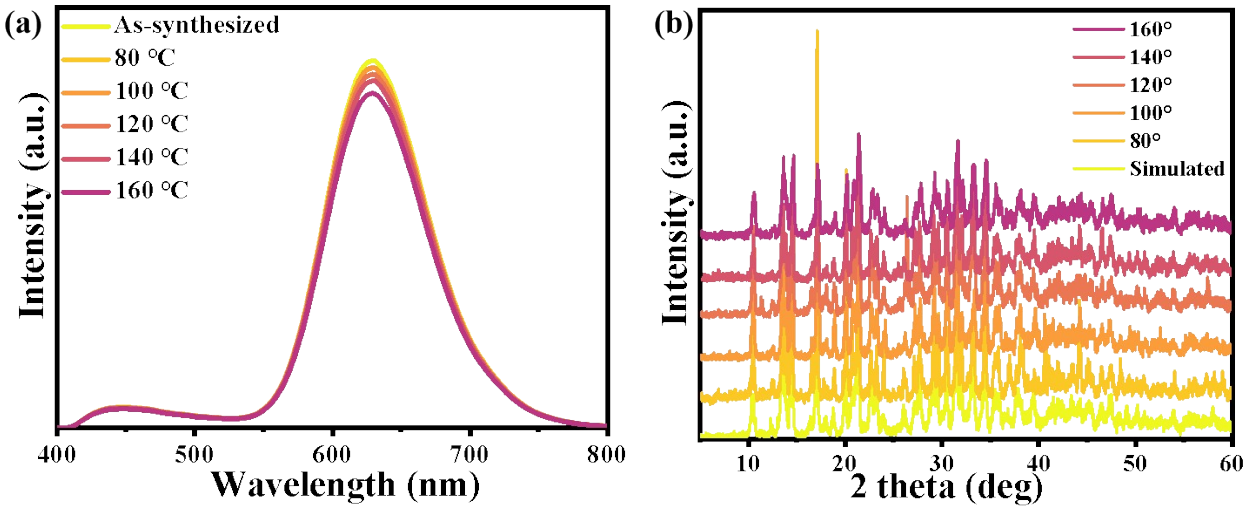


Fig. S10. The pristine and experimental emission spectra (a) and XRD patterns (b) of compound **8** after heating anneal over 10 hours.

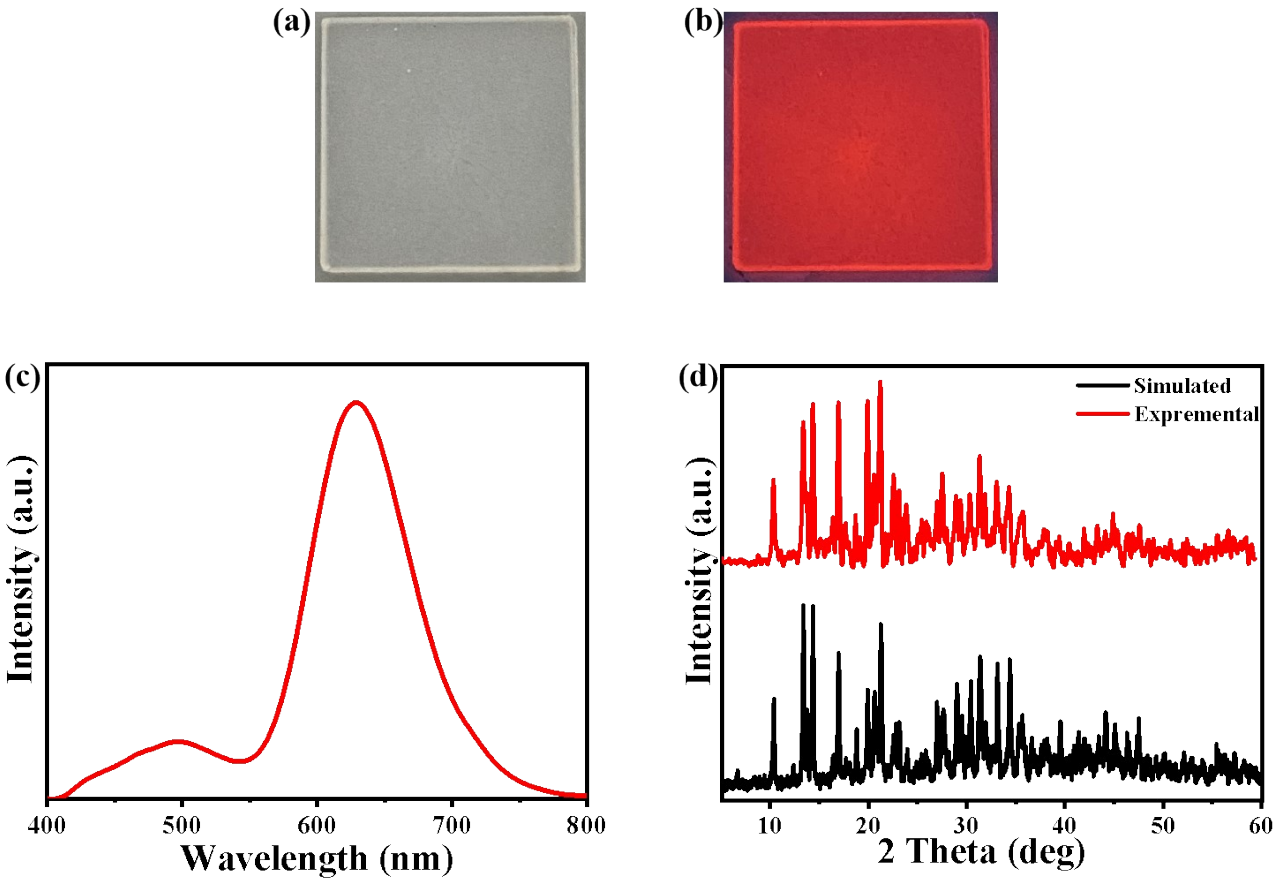


Fig. S11. The photographs of compound **8** based film under ambient light (a) and 365 nm UV light (b); the emission spectra (c) and XRD patterns (d) of compound **8** based film.

Table S1. Crystal Data and Structural Refinements for compound **1**.

Compound	**1**
chemical formula	$C_{12}H_{38}N_6Pb_2Cl_{10}O$
fw	1051.36
Space group	$P2_1/c$
crystal system	Monoclinic system
a/Å	13.4649(6)
b/Å	17.1481(8)
c/Å	13.2881(6)

α/°	90
β/°	96.1950(6)
γ/°	90
V(Å^3)	3050.3(2)
Z	4
D_{calcd} (g·cm^{-3})	2.289
Temp (K)	296(2)
μ (mm^{-1})	11.919
F(000)	1976.0
Reflections collected	36103
Unique reflections	7032
Reflections ($I>2\sigma(I)$)	5990
GOF on F^2	1.014
R_1,wR_2 ($I > 2\sigma(I)$)[a]	0.0211/0. 0400
R_1,wR_2 (all data)	0.0298/0.0419
$\Delta\rho_{max}$ (e/Å^3)	0.96
$\Delta\rho_{min}$ (e/Å^3)	-0.57
CCDC number	2252459

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$, $wR_2 = \{\sum w[(F_o)^2 - (F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$

Table S2. Selected bond lengths (Å) and bond angles (°) for compound **1**.

Pb(1)-Cl(3)	2.9409(10)	Cl(9)-Pb(1)-Cl(10)	79.80(3)
Pb(1)-Cl(4)	3.05845(17)	Cl(10)-Pb(1)-Cl(3)	175.76(3)
Pb(1)-Cl(7)	2.8695(9)	Cl(10)-Pb(1)-Cl(4)	84.910(19)
Pb(1)-Cl(8)	2.8156(10)	Cl(10)-Pb(1)-Cl(7)	91.44(3)
Pb(1)-Cl(9)	2.8075(10)	Cl(10)-Pb(1)-Cl(8)	96.90(3)
Pb(1)-Cl(10)	2.8083(9)	Cl(1)-Pb(2)-Cl(2)	90.11(2)
Pb(2)-Cl(1)	2.90264(16)	Cl(1)-Pb(2)-Cl(3)	96.79(2)
Pb(2)-Cl(2)	3.0071(11)	Cl(3)-Pb(2)-Cl(2)	94.74(3)
Pb(2)-Cl(3)	2.9965(10)	Cl(5)-Pb(2)-Cl(1)	90.32(3)
Pb(2)-Cl(5)	2.7713(10)	Cl(5)-Pb(2)-Cl(2)	171.77(3)
Pb(2)-Cl(6)	2.7757(9)	Cl(5)-Pb(2)-Cl(3)	93.37(3)
Pb(2)-Cl(11)	2.8167(8)	Cl(5)-Pb(2)-Cl(6)	87.27(3)
		Cl(5)-Pb(2)-Cl(11)	88.75(3)
Cl(3)-Pb(1)-Cl(4)	98.71(2)	Cl(1)-Pb(2)-Cl(6)	176.33(2)
Cl(3)-Pb(1)-Cl(7)	86.67(3)	Cl(6)-Pb(2)-Cl(2)	91.88(3)
Cl(7)-Pb(1)-Cl(4)	85.464(19)	Cl(6)-Pb(2)-Cl(3)	86.12(3)
Cl(3)-Pb(1)-Cl(8)	85.39(3)	Cl(6)-Pb(2)-Cl(11)	82.87(3)
Cl(8)-Pb(1)-Cl(4)	89.37(2)	Cl(11)-Pb(2)-Cl(1)	94.313(19)
Cl(8)-Pb(1)-Cl(7)	169.77(3)	Cl(11)-Pb(2)-Cl(2)	83.02(3)
Cl(3)-Pb(1)-Cl(9)	96.46(3)	Cl(11)-Pb(2)-Cl(3)	168.68(3)
Cl(9)-Pb(1)-Cl(4)	164.39(2)	Pb(2)-Cl(1)-Pb(2)#1	180
Cl(9)-Pb(1)-Cl(7)	91.78(3)	Pb(1)-Cl(3)-Pb(2)	169.03(4)
Cl(9)-Pb(1)-Cl(8)	95.51(3)	Pb(1)#2-Cl(1)-Pb(1)	180

Symmetry transformations used to generate equivalent atoms: #1 2-*x*, -*y*, 2-*z*, #2 1-*x*, -*y*, 1-*z*

Table S3. Hydrogen bonds data for compound **1**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A)···Cl(2)	0.89	2.230	3.053	153.49
N(1)-H(1B)···Cl(1)	0.89	2.631	3.454	154.22
N(1)-H(1C)···Cl(6)	0.89	2.193	3.062	165.30
N(1a)-H(1aB)···Cl(11)	0.89	2.894	3.435	120.74
N(1a)-H(1aB)···Cl(2)	0.89	2.280	3.146	164.04
N(1a)-H(1aB)···Cl(6)	0.89	2.509	3.307	149.57
N(4)-H(4A)···O(1)	0.89	1.934	2.805	165.80
N(4)-H(4B)···Cl(8)	0.89	2.435	3.278	158.17
N(5)-H(5)···Cl(6)	0.98	2.585	3.295	129.46
N(5)-H(5)···Cl(11)	0.98	2.544	3.338	138.11
C(1)-H(1E)···Cl(4)	0.97	2.889	3.673	138.61
C(1)-H(1E)···Cl(7)	0.97	2.779	3.471	128.84
C(2)-H(2B)···Cl(8)	0.97	2.931	3.689	135.80
C(3)-H(3A)···Cl(5)	0.97	2.842	3.771	160.45
C(3)-H(3A)···Cl(6)	0.97	2.749	3.264	113.83
C(3)-H(3B)···Cl(8)	0.97	2.783	3.583	140.29
C(3)-H(3B)···Cl(11)	0.97	2.917	3.66	134.16
C(4)-H(4C)···Cl(2)	0.97	2.891	3.715	143.34
C(4)-H(4D)···Cl(6)	0.97	2.864	3.496	123.66
C(16)-H(16A)···Cl(3)	0.97	2.683	3.646	172.20
C(16)-H(16B)···Cl(11)	0.97	2.800	3.671	149.86
C(16a)-H(16C)···Cl(1)	0.97	2.731	3.469	133.27
C(16a)-H(16D)···Cl(5)	0.97	2.916	3.871	168.37
C(17)-H(17A)···Cl(9)	0.97	2.986	3.869	151.88
C(17)-H(17B)···Cl(11)	0.97	2.866	3.775	156.42
C(17)-H(17C)···Cl(11)	0.97	2.898	3.775	150.91
C(17)-H(17D)···Cl(8)	0.97	2.867	3.798	161.08
N(2)-H(2C)···Cl(10)	0.89	2.338	3.213	167.79

N(2)-H(2D)···Cl(11)	0.89	2.333	3.202	165.59
N(2)-H(2E)···Cl(9)	0.89	2.373	3.170	149.15
N(3)-H(3C)···Cl(7)	0.89	2.397	3.184	147.49
N(3)-H(3D)···O(1)	0.89	1.949	2.837	175.09
N(6)-H(6)···Cl(9)	0.98	2.481	3.25	135.11
N(6)-H(6)···Cl(10)	0.98	2.573	3.323	133.36
C(5)-H(5B)···Cl(7)	0.97	2.85	3.676	143.48
C(7)-H(7B)···Cl(2)	0.97	2.902	3.768	149.15
C(8)-H(8A)···Cl(10)	0.97	2.719	3.437	131.23
C(8)-H(8B)···Cl(5)	0.97	2.96	3.768	141.56
C(9)-H(9A)···Cl(5)	0.97	2.96	3.818	148.10
C(9)-H(9A)···Cl(6)	0.97	2.914	3.589	127.61
C(10)-H(10A)···Cl(7)	0.97	2.87	3.684	142.04
C(10)-H(10B)···Cl(5)	0.97	2.816	3.705	152.65
C(18)-H(18A)···Cl(4)	0.97	2.936	3.679	134.21
C(18)-H(18A)···Cl(8)	0.97	2.884	3.610	132.44

Table S4. Detail of one-pot synthesis of Mn^{2+}-doped 1D lead chloride crystals.

Product	$PbCl_2$ (mmol)	$MnCl_2·4H_2O$ (mmol)	$C_6H_{15}N_3$ (mmol)
compound **2**	0.5	0.1	0.6
compound **3**	0.5	0.2	0.6
compound **4**	0.5	0.3	0.6
compound **5**	0.5	0.4	0.6
compound **6**	0.5	0.5	0.6
compound **7**	0.5	0.6	0.6
compound **8**	0.5	0.7	0.6

compound **9**	0.5	0.8	0.6