Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

A Thermally Induced Fluorescence Enhancement Strategy for Efficient All-Inorganic Rubidium Manganese Halides

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Table S1. The lattice parameters of $Rb_2MnBr_4 \cdot 2H_2O$.

Atom	Position	x	y	z	Ueq(Å^2)	Occupancy
Rb1	2i	0.24252(25)	0.15534(16)	0.12391(16)	0.0342(3)	1
Br1	2i	0.75687(25)	0.87839(16)	0.38181(16)	0.0408(3)	1
Br2	2i	0.26293(25)	0.64119(16)	0.16331(16)	0.0515(0)	1
O1	2i	0.76503(25)	0.36858(16)	0.33953(16)	0.0097(0)	1
Mn1	1g	0	0.50000	0.50000	0.3113(3)	1
Space group: P-1 (No. 2), triclinic, Z=1, α=66.0032(7)°, β=87.7903(14)°, γ=84.8967(14)°						
Cell parameters		a= 5.8916(0) Å、 b= 6.8800(1) Å、 c= 7.3647(1) Å and V= 271.64(1) Å^3				
Reliability factor:		R_{wp}=11.68%, R_p=8.36%, χ^2=1.82				

Table S2. The EDS analysis of $Rb_2MnBr_4 \cdot 2H_2O$ with different temperature treatment.

Sample with different temperature treatment	Rb/(Atomic %)	Mn/(Atomic %)	Br/(Atomic %)	O/(Atomic %)
30 ℃	26.02	8.70	40.68	24.59
160 ℃	30.91	10.41	46.40	12.28

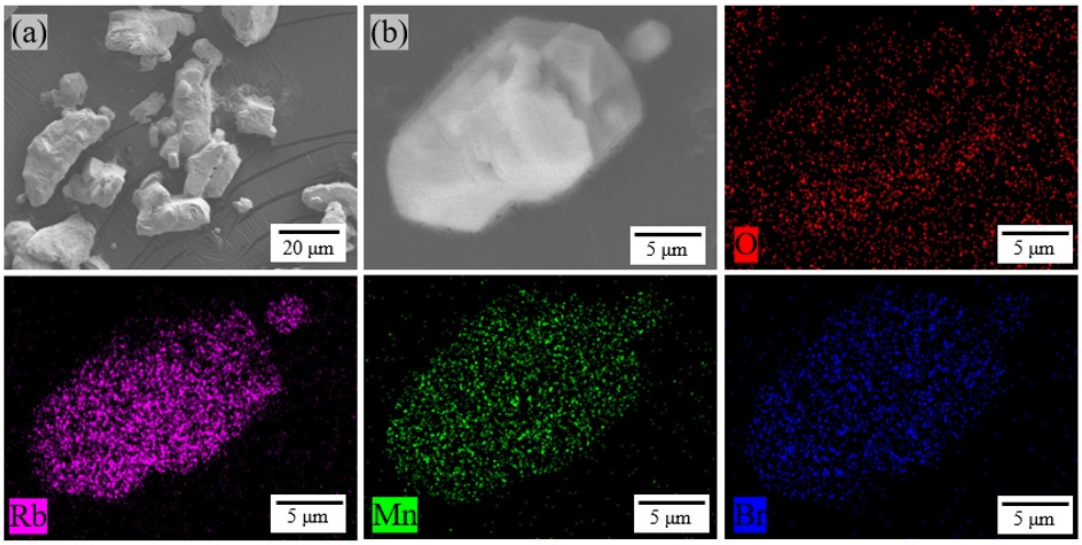

Fig. S1 (a) SEM images and (b) EDS mapping of $Rb_2MnBr_4{\cdot}2H_2O$.

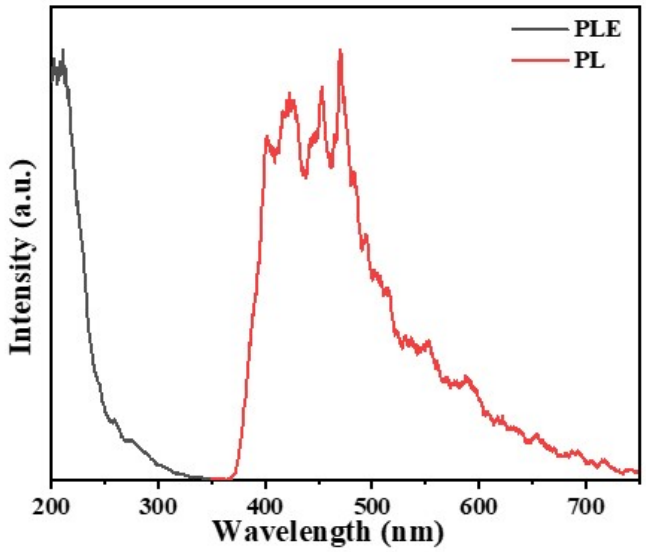

Fig. S2 PLE and PL spectra of $Rb_2MnBr_4{\cdot}2H_2O$ at room temperature.

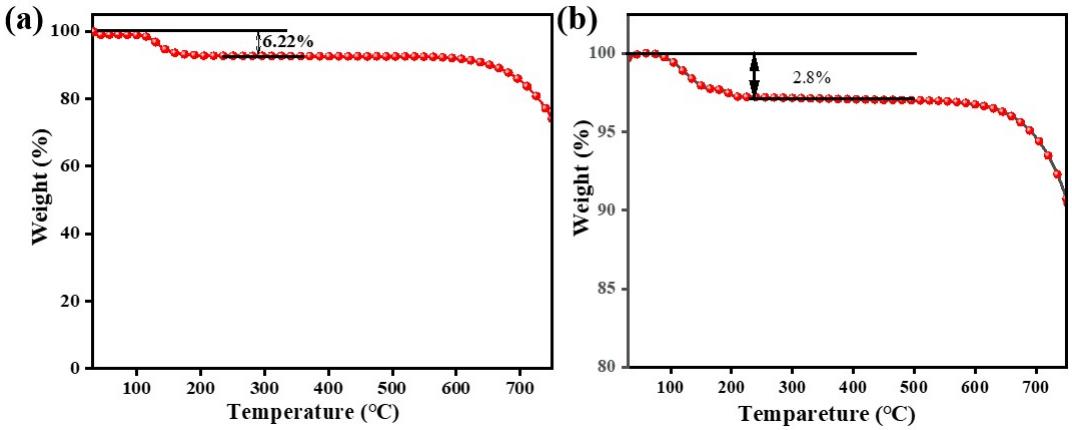

Fig. S3 TGA curves of (a) $Rb_2MnBr_4{\cdot}2H_2O$ and (b) $Rb_2MnBr_4{\cdot}2H_2O$ after 160 ℃ treatment.

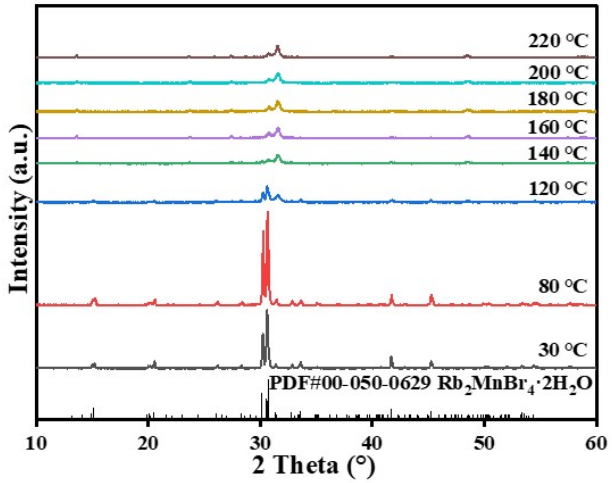

Fig. S4 Temperature-dependent XRD patterns of $Rb_2MnBr_4{\cdot}2H_2O$ crystals.

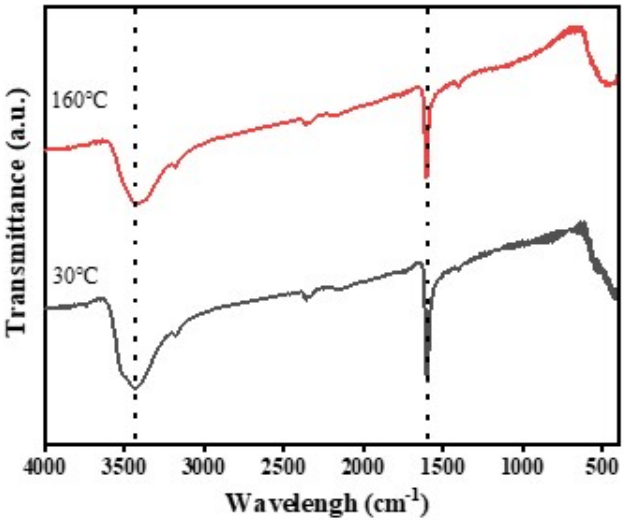

Fig. S5 FT-IR spectra of $Rb_2MnBr_4{\cdot}2H_2O$ crystals with different temperature.

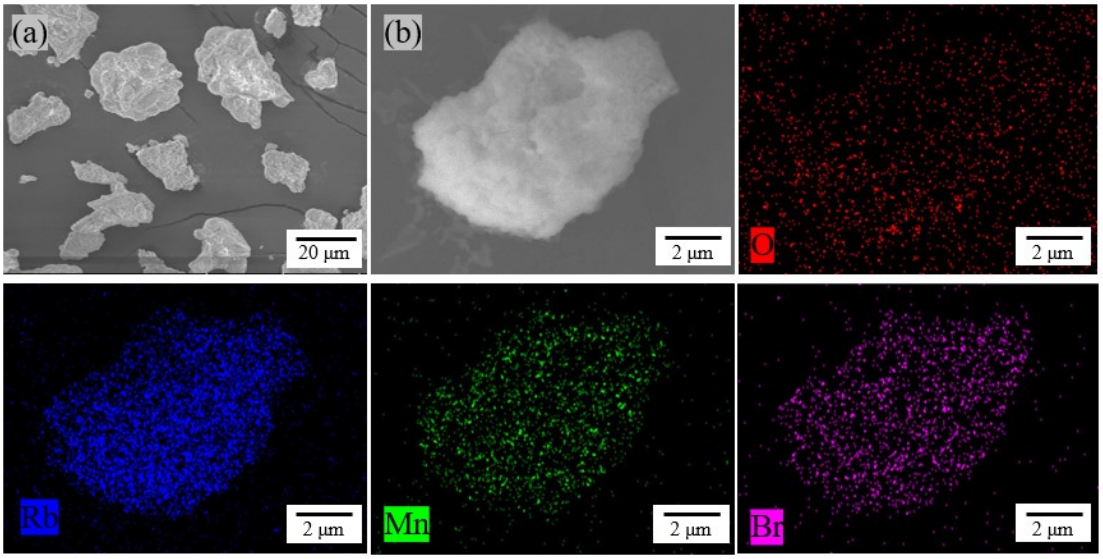

Fig. S6 (a) SEM images and (b) EDS mapping of $Rb_2MnBr_4{\cdot}2H_2O$ after heat treatment at 160 ℃.

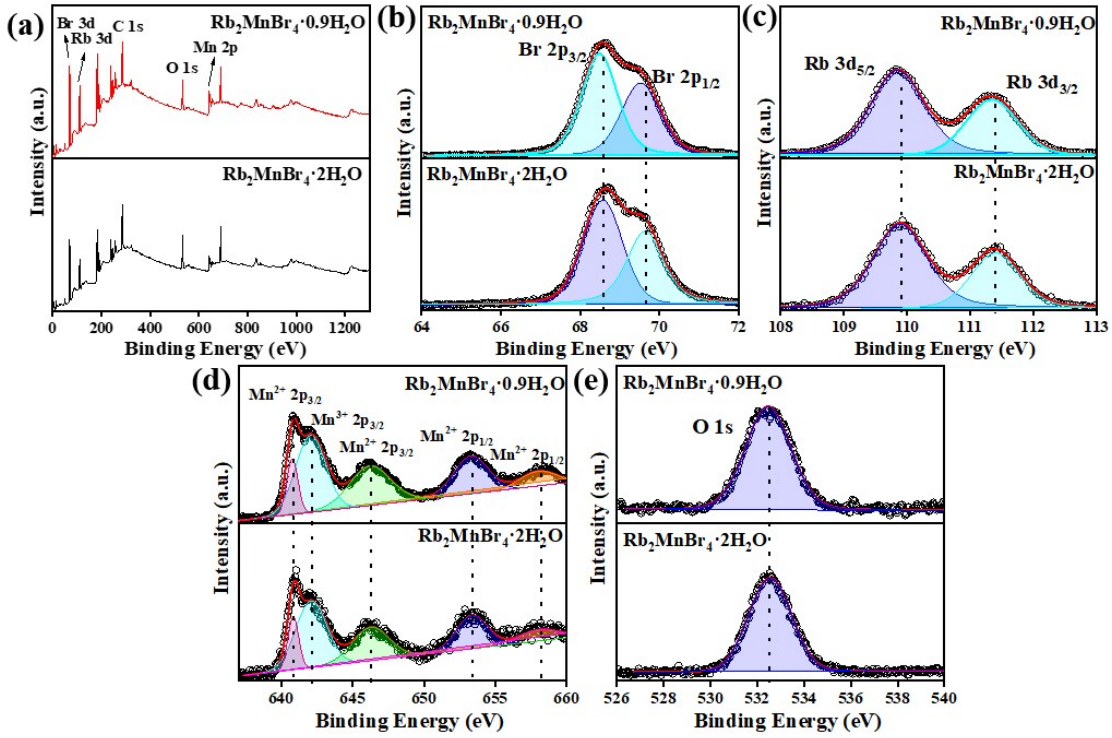

Fig. S7 (a) XPS survey, high-resolution spectra of (b) Br 2p, (c) Rb 3d, (d) Mn 2p and (e) O 1s for $Rb_2MnBr_4{\cdot}0.9\ H_2O$ and $Rb_2MnBr_4{\cdot}2H_2O$.

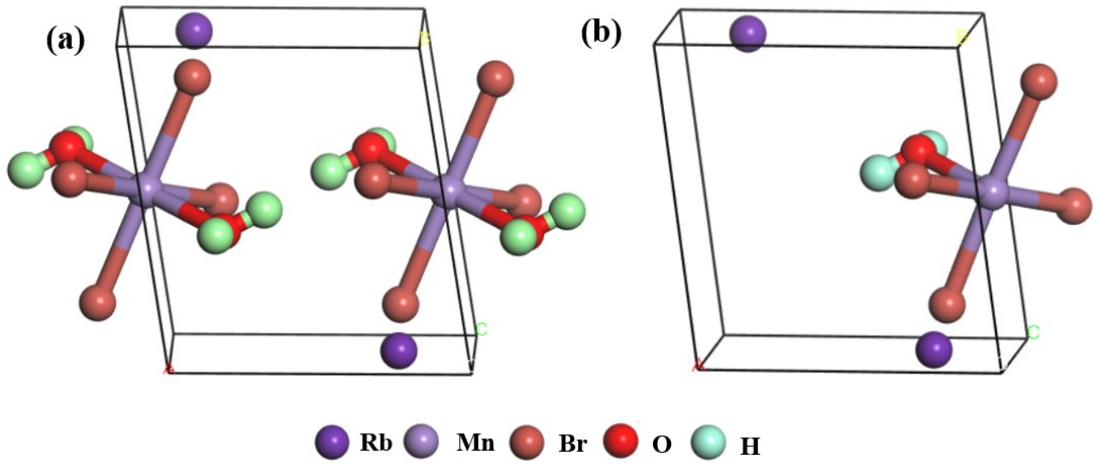

Fig. S8 Optimized structures of (a) $Rb_2MnBr_4{\cdot}2H_2O$ and (b) $Rb_2MnBr_4{\cdot}1H_2O$.

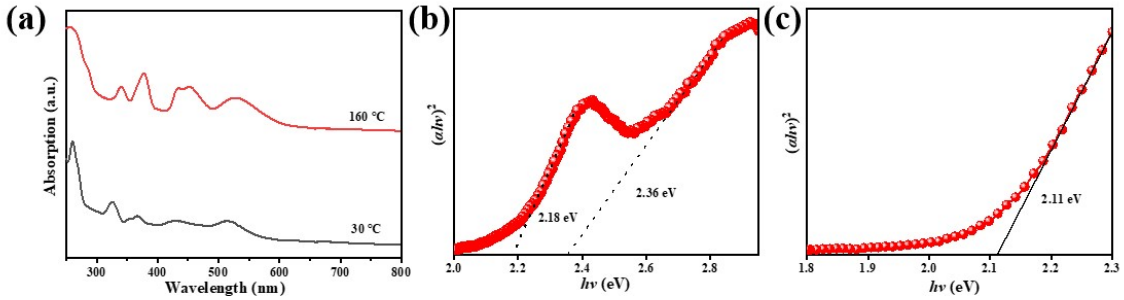

Fig. S9 (a) Absorption spectra of $Rb_2MnBr_4{\cdot}2H_2O$ after heat treatment at 30 ℃ and 160 ℃, the fitted band gap of $Rb_2MnBr_4{\cdot}2H_2O$ after heat treatment at (b) 30 ℃ and (c) 160 ℃ by the Tauc plot method.

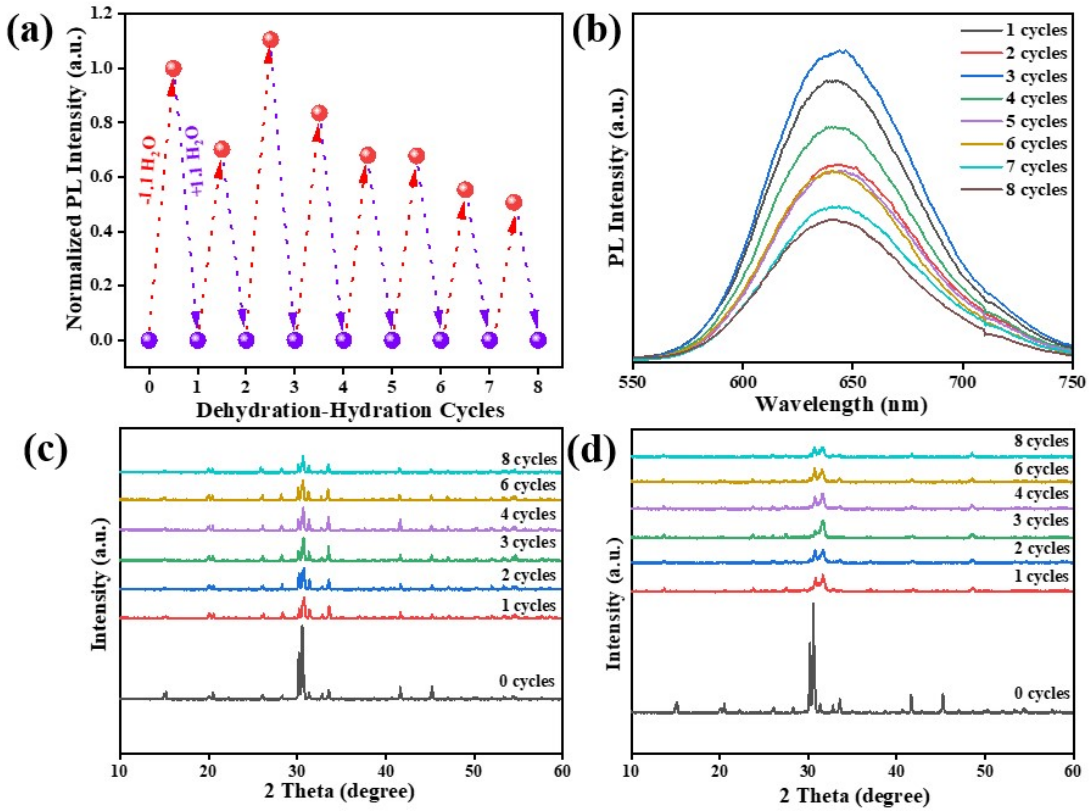

Fig. S10 (a) Normalized PL intensity of $Rb_2MnBr_4{\cdot}2H_2O$ in the dehydration-hydration cycles, (b) PL spectra of $Rb_2MnBr_4{\cdot}2H_2O$ in dehydration cycles, XRD pattern of $Rb_2MnBr_4{\cdot}2H_2O$ in (c) hydration cycles and (d) dehydration cycles.

The calculations of crystal field (Δ) are based on Tanabe-Sugano energy diagram of d^5 electronic configurations, which can be obtained by the following equation (Eqs. (1)–(4)):

$$\Delta=10D_q \quad (1)$$

$$^6A_1(^6S) \rightarrow [^4E(^4G), {}^4A_1(^4G)] =10B+5C+20\alpha \quad (2)$$

$$^6A_1(^6S) \rightarrow {}^4E(^4D) =17B+5C+6\alpha \quad (3)$$

$$^6A_1(^6S) \rightarrow {}^4T_2(^4D) =13B+5C+8\alpha \quad (4)$$

$$^6A_1(^6S) \rightarrow {}^4T_2(^4G) =-10D_q+18B+6C-(26B^2/10D_q)+22\alpha \quad (5)$$

The $^6A_1(^6S) \rightarrow [^4E(^4G), {}^4A_1(^4G)]$, $^6A_1(^6S) \rightarrow {}^4E(^4D)$, $^6A_1(^6S) \rightarrow {}^4T_2(^4D)$ and $^6A_1(^6S) \rightarrow {}^4T_2(^4G)$ can be obtained via converting the PLE into the diagram of energy coordinates.