

Electronic Supplementary Information

Insights into luminescence thermal quenching of Mn⁴⁺-doped BaLa(Na/Li)(W/Te)O₆ double perovskite red phosphors

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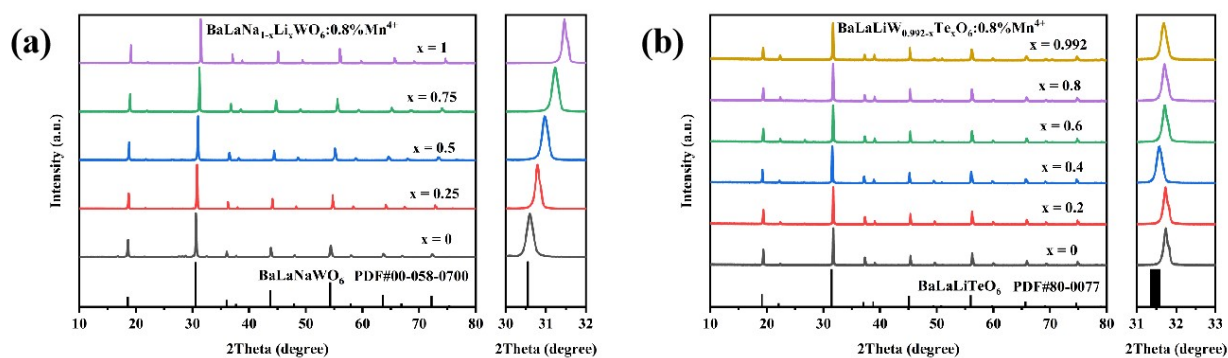


Figure S1: XRD patterns of synthesized (a) BaLaNa_{1-x}Li_xWO₆:0.8%Mn⁴⁺ and (b) BaLaLiW_{0.992-x}Te_xO₆:0.8%Mn⁴⁺.

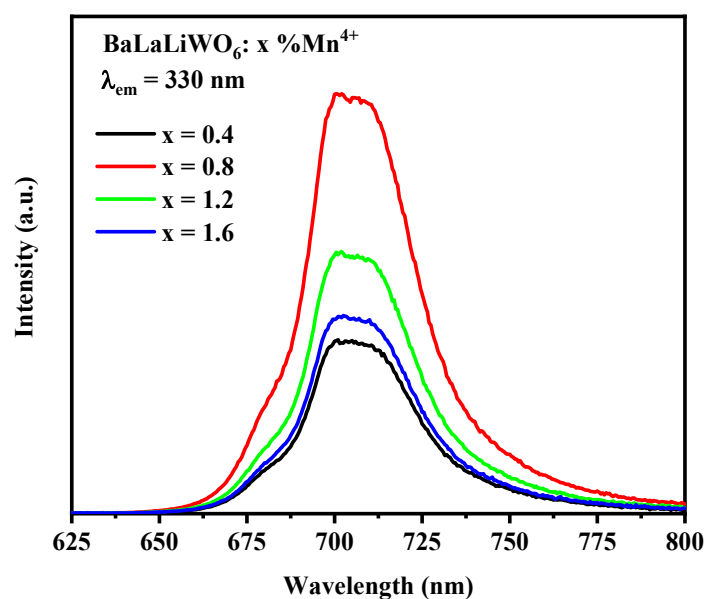


Figure S2: PL spectra of BaLaLiWO₆:x %Mn⁴⁺ (x = 0.4, 0.8, 1.2, 1.6) upon Mn⁴⁺ excitation at 330 nm

Table S1: Fractional atomic coordinates and isotropic displacement parameters of

BaLaNaWO ₆ :0.8%Mn ⁴⁺					
	x	y	z	B	Occ
Ba	0.25000	0.25000	0.25000	0.300	0.500
La	0.25000	0.25000	0.25000	0.300	0.500
Na	0.00000	0.00000	0.00000	1.000	1.000
W	0.50000	0.50000	0.50000	0.200	0.990
Mn	0.50000	0.50000	0.50000	0.200	0.010
O	0.26500	0.00000	0.00000	1.500	1.000

Table S2: Fractional atomic coordinates and isotropic displacement parameters of

BaLaLiWO ₆ :0.8%Mn ⁴⁺					
	x	y	z	B	Occ
Ba	0.25000	0.25000	0.25000	0.300	0.500
La	0.25000	0.25000	0.25000	0.300	0.500
Li	0.00000	0.00000	0.00000	1.000	1.000
W	0.50000	0.50000	0.50000	0.200	0.990
Mn	0.50000	0.50000	0.50000	0.200	0.010
O	0.26001	0.00000	0.00000	1.500	1.000

Table S3: Fractional atomic coordinates and isotropic displacement parameters of

BaLaLiTeO₆:0.8%Mn⁴⁺

	x	y	z	B	Occ
Ba	0.25000	0.25000	0.25000	0.300	0.500
La	0.25000	0.25000	0.25000	0.300	0.500
Li	0.00000	0.00000	0.00000	1.000	1.000
Te	0.50000	0.50000	0.50000	0.200	0.990
Mn	0.50000	0.50000	0.50000	0.200	0.010
O	0.26151	0.00000	0.00000	1.500	1.000

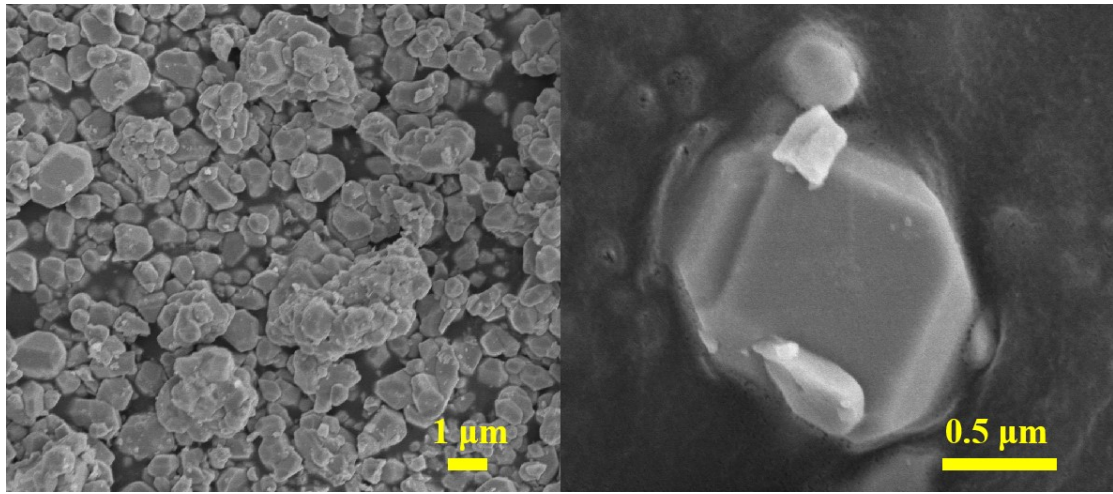


Figure S3: SEM images of the as-prepared BaLaLiTeO₆:0.8%Mn⁴⁺.

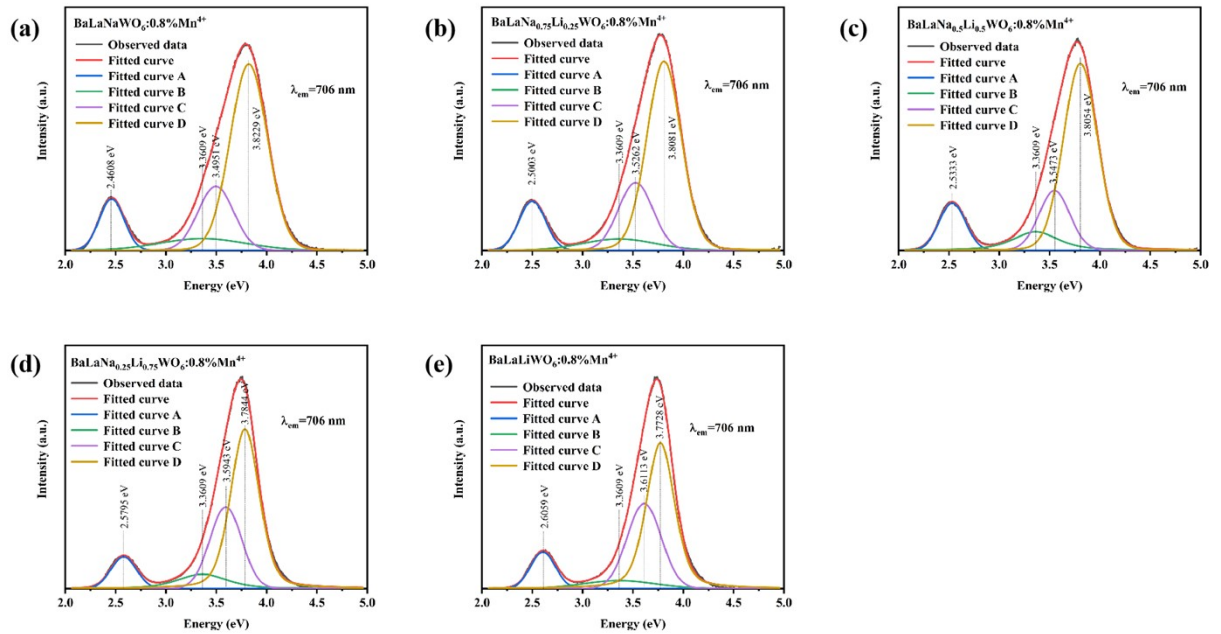
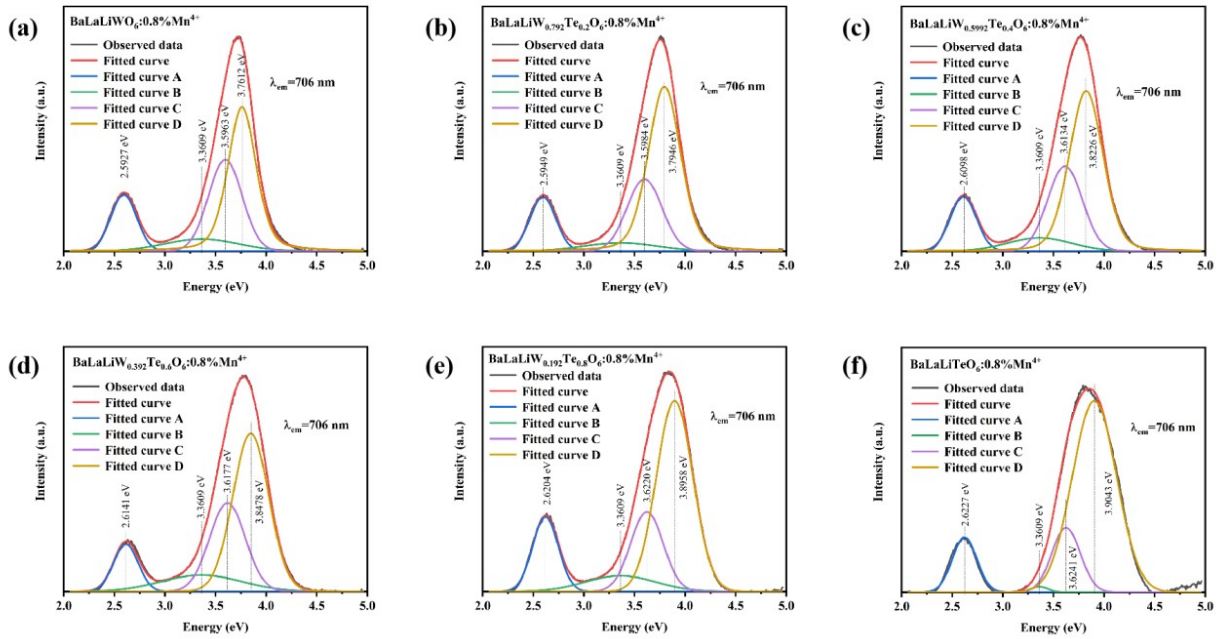


Figure S4: Gaussian fitting of BaLaNa_{1-x}Li_xWO₆:0.8%Mn⁴⁺ PLE spectra

(a) x = 0; (b) x = 0.25; (c) x = 0.5; (d) x = 0.75; (e) x = 1.

Table S4: Position of each transition energy level in the excitation spectra of BaLaNa_{1-x}Li_xWO₆:0.8 %Mn⁴⁺ obtained by Gaussian fitting

	${}^4A_{2g} \rightarrow {}^4T_{2g}$ (eV)	${}^4A_{2g} \rightarrow {}^2T_{2g}$ (eV)	${}^4A_{2g} \rightarrow {}^4T_{1g}$ (eV)	Mn ⁴⁺ -O ²⁻ (eV)
x=0	2.461	3.361	3.495	3.823
x=0.25	2.500	3.361	3.526	3.808
x=0.5	2.533	3.361	3.547	3.805
x=0.75	2.580	3.361	3.594	3.784
x=1	2.606	3.361	3.611	3.773

**Figure S5:** Gaussian function of PLE spectra of BaLaLiW_{0.992-x}Te_xO₆:0.8%Mn⁴⁺ samples (a) x = 0; (b) x = 0.2; (c) x = 0.4; (d) x = 0.6; (e) x = 0.8; (e) x = 1.**Table S5:** Energy of Mn⁴⁺ related transitions observed in BaLaLiW_{0.992-x}Te_xO₆:0.8 %Mn⁴⁺ as obtained by Gaussian fitting

${}^4A_{2g} \rightarrow {}^4T_{2g}$ (eV)	${}^4A_{2g} \rightarrow {}^2T_{2g}$ (eV)	${}^4A_{2g} \rightarrow {}^4T_{1g}$ (eV)	Mn ⁴⁺ -O ²⁻ (eV)
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x=0	2.593	3.361	3.596	3.761
x=0.2	2.595	3.361	3.598	3.795
x=0.4	2.610	3.361	3.613	3.823
x=0.6	2.614	3.361	3.618	3.848
x=0.8	2.620	3.361	3.622	3.896
x=0.992	2.623	3.361	3.624	3.904

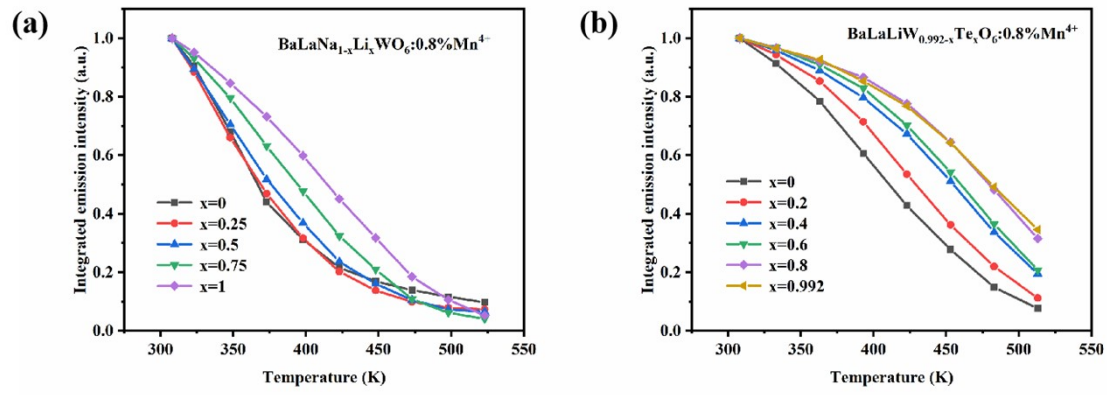


Figure S6: Temperature-dependent integrated emission intensity of (a) BaLaNa_{1-x}Li_xWO₆:0.8%Mn⁴⁺ and (b) BaLaLiW_{0.992-x}Te_xO₆:0.8%Mn⁴⁺.

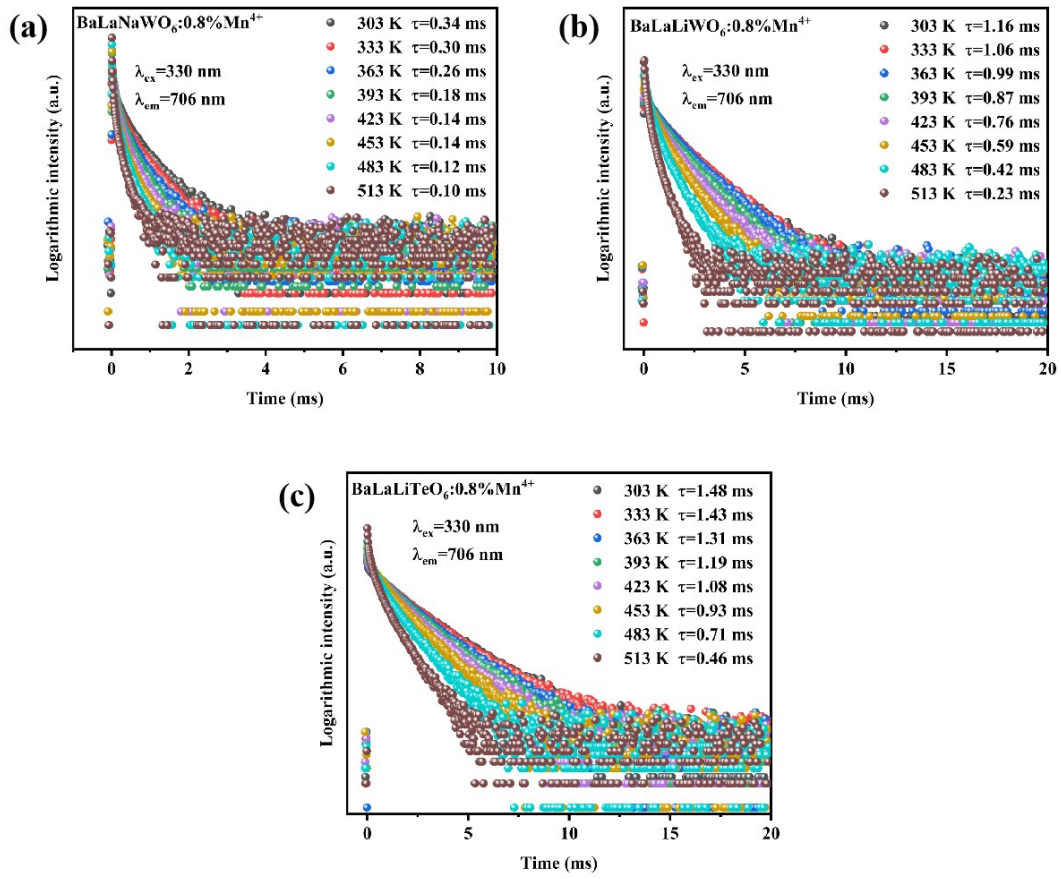


Figure S7: Temperature-dependent decay curves of $\text{Mn}^{4+} {}^2E_g$ state in (a) $\text{BaLaNaWO}_6:0.8\%\text{Mn}^{4+}$ (b) $\text{BaLaLiWO}_6:0.8\%\text{Mn}^{4+}$ and (c) $\text{BaLaLiTeO}_6:0.8\%\text{Mn}^{4+}$ upon excitation at 330 nm.

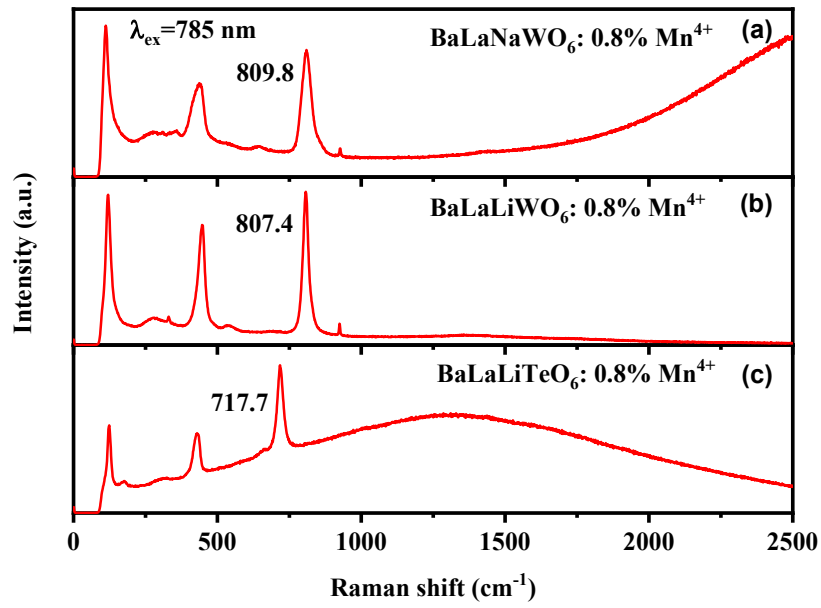


Figure S8: Raman spectra of (a) $\text{BaLaNaWO}_6:0.8\%\text{Mn}^{4+}$ (b) $\text{BaLaLiWO}_6:0.8\%\text{Mn}^{4+}$ and (c) $\text{BaLaLiTeO}_6:0.8\%\text{Mn}^{4+}$.