

Supplementary Material

Energy Transfer Induced Blue-Light Excited Broadband Near-infrared

Luminescence in Fluoride $\text{Na}_3\text{AlF}_6:\text{Mn}^{4+},\text{Fe}^{3+}$

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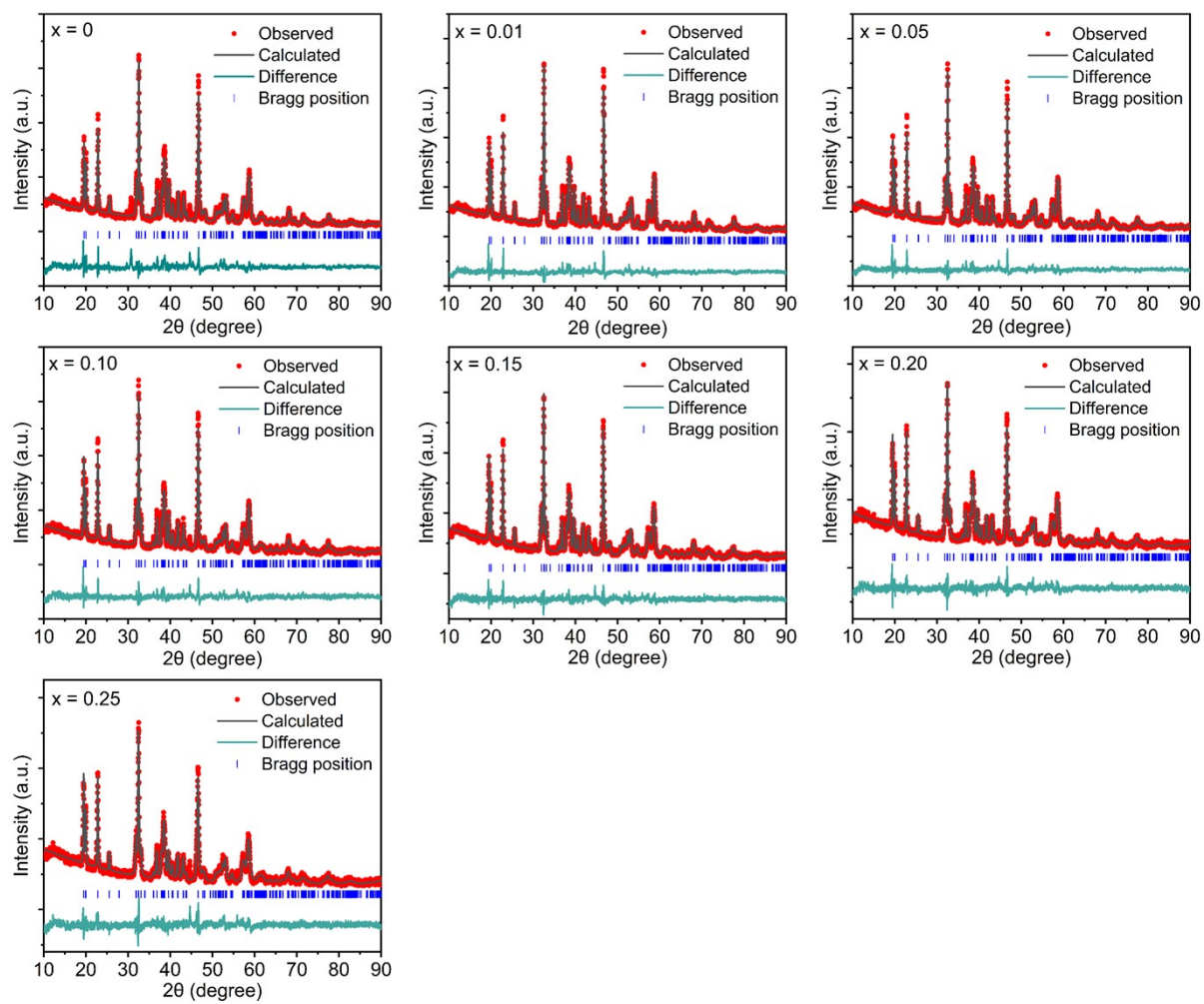


Fig. S1. Rietveld refinement results of NAF:0.03Mn⁴⁺, xFe³⁺ (x = 0-0.25).

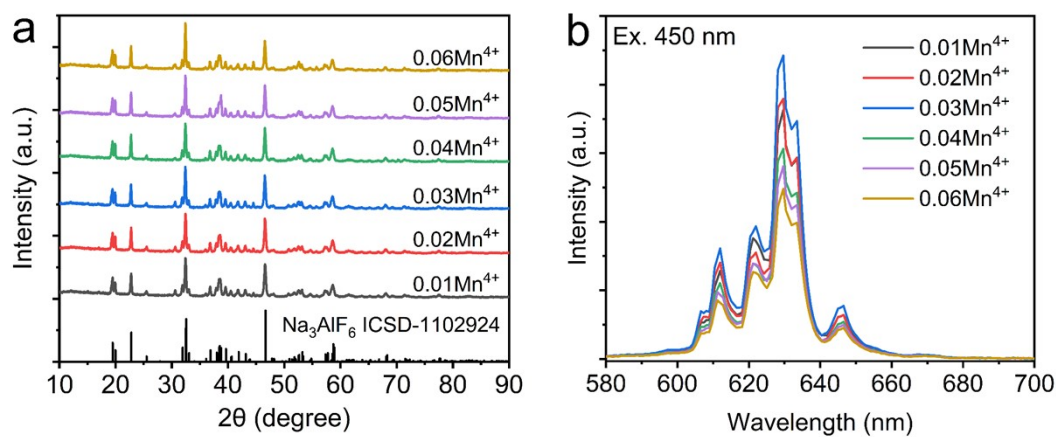


Fig. S2. (a) XRD patterns and (b) emission spectra of $\text{Na}_3\text{AlF}_6:\text{yMn}^{4+}$ ($y = 0.01-0.06$).

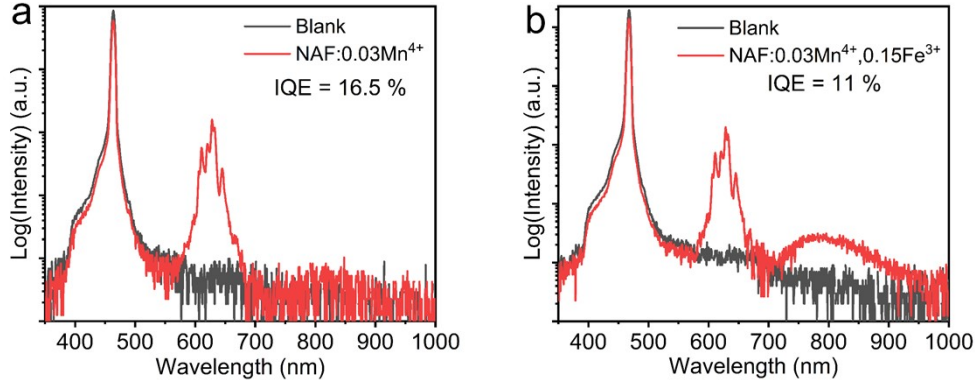


Fig. S3. The quantum efficiency results of NAF:0.03Mn⁴⁺ (a) and NAF:0.03Mn⁴⁺, 0.15Fe³⁺ (b) upon excitation at 463 nm blue light. The internal quantum efficiency (IQE) can be calculated by the following equation:

$$IQE = \frac{\int L_S}{\int E_B - E_S} \times 100\% \quad (S1)$$

where L_S means the emitted photons of the samples, E_S and E_B is the integrated area of the excitation light with and without the phosphor.

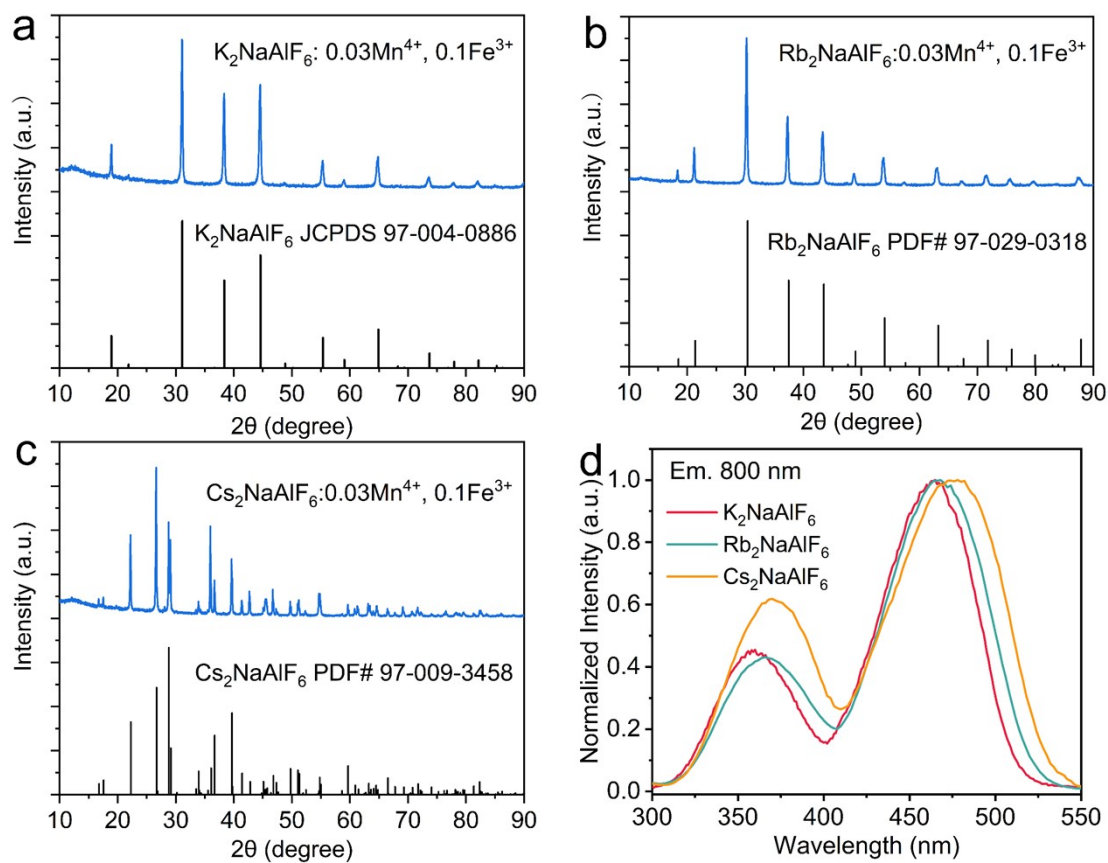


Fig. S4. (a-c) XRD patterns of $\text{K}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$, $\text{Rb}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$, $\text{Cs}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$. (b) The normalized excitation spectra of $\text{K}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$, $\text{Rb}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$, $\text{Cs}_2\text{NaAlF}_6:0.03\text{Mn}^{4+}, 0.1\text{Fe}^{3+}$.

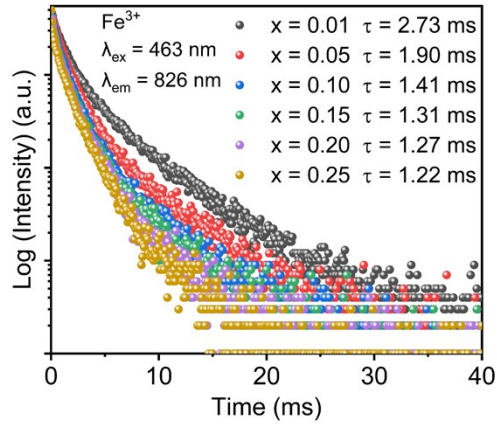


Fig. S5. The decay curves of NAF:0.03Mn⁴⁺, xFe³⁺ monitored at 826 nm. The continuous decrease lifetime with increasing Fe³⁺ concentration can be understood since concentration quenching of Fe³⁺ will result in increased non-radiative transition probability and thus the decay became faster.

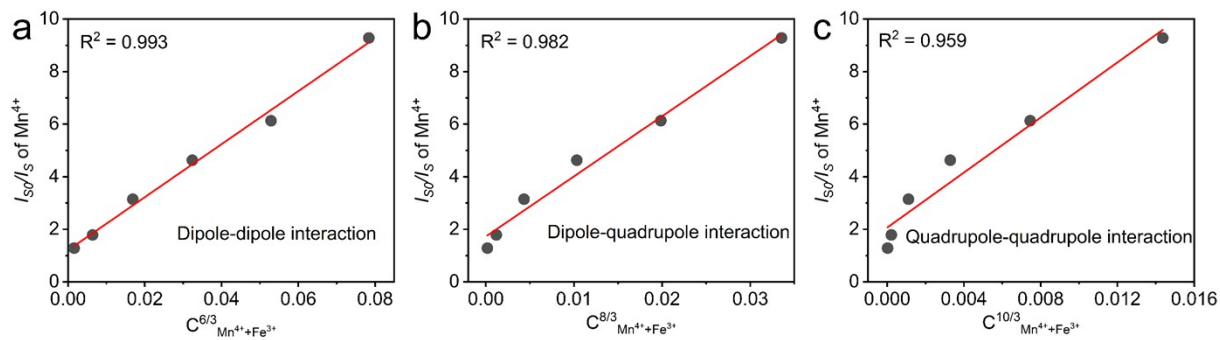


Fig. S6. I_{S0}/I_S - $C^{a/3}$ diagram of NAF:0.03 Mn^{4+} , xFe^{3+} .

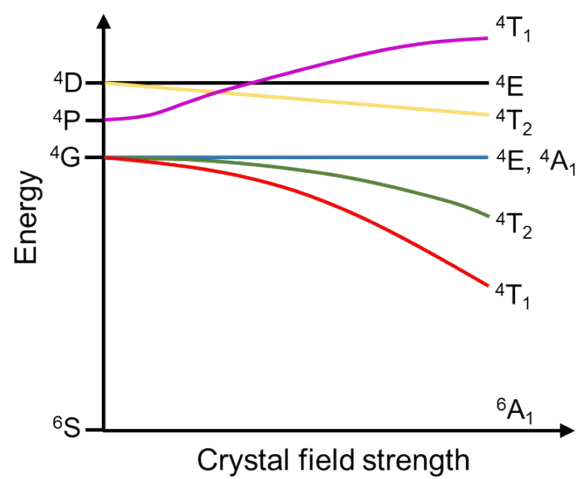


Fig. S7. The Tanabe–Sugano diagram for Fe³⁺ in an octahedral site.

Table S1. Main cell parameters of processing and refinement of the $\text{Na}_3\text{AlF}_6:0.03\text{Mn}^{4+}, x\text{Fe}^{3+}$ samples.

x (Fe^{3+})	Space group	Cell Parameters				R_p, R_{wp} (%), χ^2
		a (Å)	b (Å)	c (Å)	V (Å ³)	
0	P2 ₁ /c	5.4085	5.5988	9.46200	235.609	7.86, 10, 3.89
0.01	P2 ₁ /c	5.4099	5.5991	9.4617	235.663	7.05, 9.34, 3.09
0.05	P2 ₁ /c	5.4115	5.6021	9.4655	235.964	6.30, 8.32, 2.69
0.10	P2 ₁ /c	5.4166	5.6084	9.4748	236.711	5.99, 7.95, 2.65
0.15	P2 ₁ /c	5.4181	5.6108	9.4763	236.939	5.17, 6.68, 2.11
0.20	P2 ₁ /c	5.4202	5.6131	9.4801	237.241	5.16, 6.64, 2.17
0.25	P2 ₁ /c	5.4223	5.6159	9.4844	237.544	4.94, 6.35, 2.24

Table S2. Fractional atomic coordinates and Wyckoff sites of the $\text{Na}_3\text{AlF}_6:0.03\text{Mn}^{4+}, 0.15\text{Fe}^{3+}$ sample.

Atoms	x	y	z	Wyckoff sites	Occ.
Na1	0.27186	0.05423	0.75375	4e	1
Na2	0.5	0	0.5	2d	1
Al1	0	0	0	2a	0.82
Mn1	0	0	0	2a	0.03
Fe1	0	0	0	2a	0.15
F1	0.11350	0.04448	0.21906	4e	1
F2	0.22960	0.73172	0.06265	4e	1
F3	0.32695	0.17715	0.04772	4e	1

Table S3. The excitation peak wavelength (λ_{ex}), emission peak wavelength (λ_{em}) and FWHM values of Fe³⁺-doped phosphors.

Phosphors	λ_{ex} (nm)	λ_{em} (nm)	FWHM (nm)	Ref.
KAl ₁₁ O ₁₇ :Fe ³⁺	340	770	-	1
Ca ₂ InSbO ₆ :Fe ³⁺	340	935	126	2
Ca ₂ LuSbO ₆ :Fe ³⁺	336	927	128	3
Ca ₂ YSbO ₆ :Fe ³⁺	345	938	135	
SrAl ₁₂ O ₁₉ : Fe ³⁺	270	812	-	4
CaAl ₁₂ O ₁₉ :Fe ³⁺	260	810	-	5
LiAl ₅ O ₈ :Fe ³⁺	284	673	-	6
NaAl ₅ O ₈ :Fe ³⁺	346	754	-	7
NaScSi ₂ O ₆ :Fe ³⁺	300	900	135	8
Sr ₉ Ga(PO ₄) ₇ :Fe ³⁺	330	915	155	9
ZnGa ₂ O ₄ :Fe ³⁺	344	720	70	10
BaSnO ₃ :Fe ³⁺	380	896	105	11
NAF:Mn ⁴⁺ , Fe ³⁺	463	826	127	This work

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