

**Cr³⁺-activated Na₃X₂Li₃F₁₂ (X=Al, Ga, In) garnet phosphors with
broadband NIR emission and high luminescence efficiency for
potential biomedical application**

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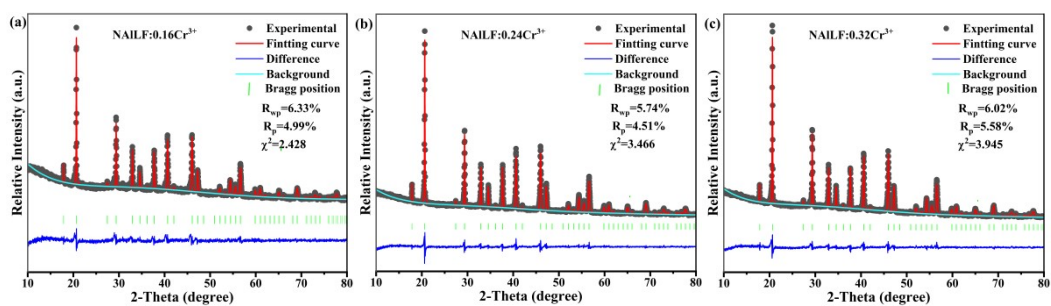
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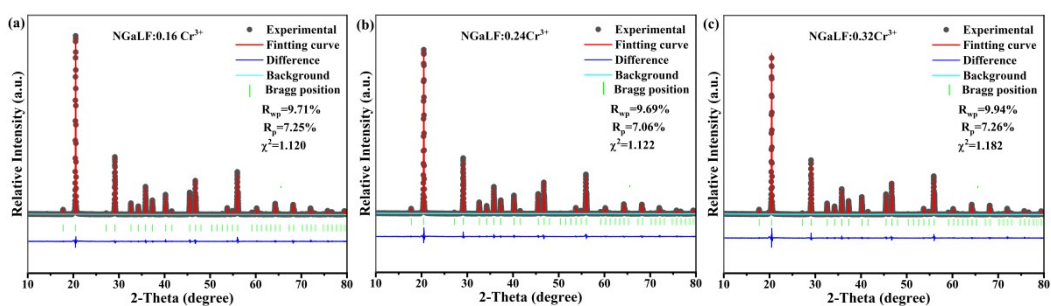
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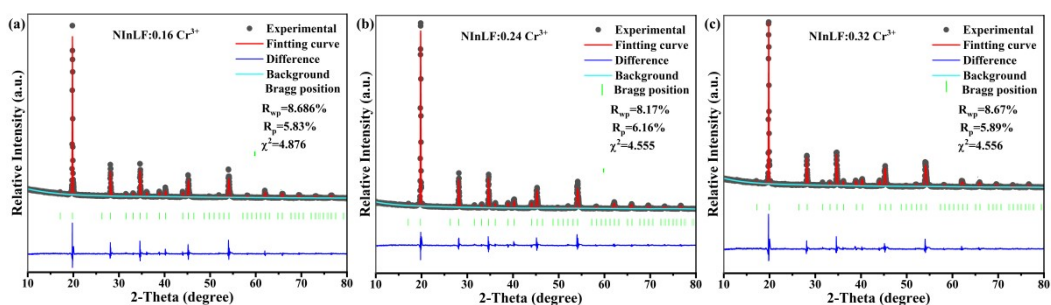
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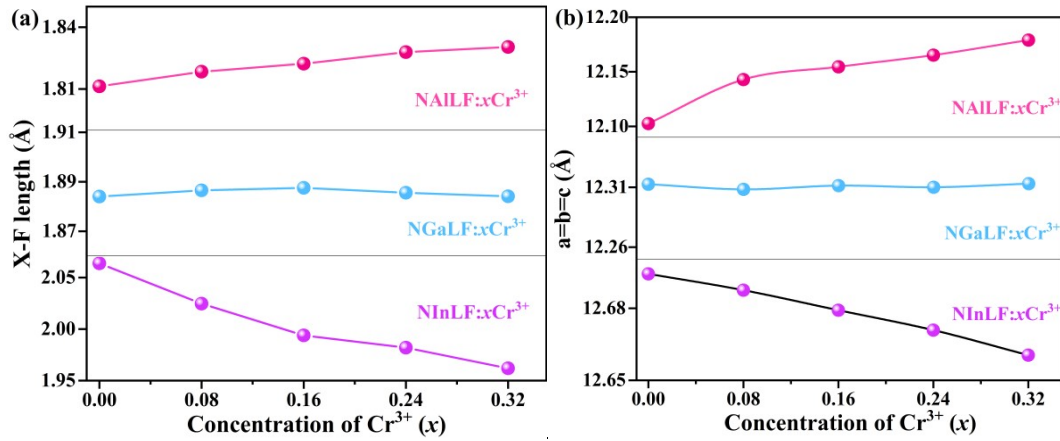
S1 Rietveld refinements of NAILF:0.16Cr³⁺ (a), NAILF:0.24Cr³⁺ (b) and NAILF:0.32Cr³⁺ (c).



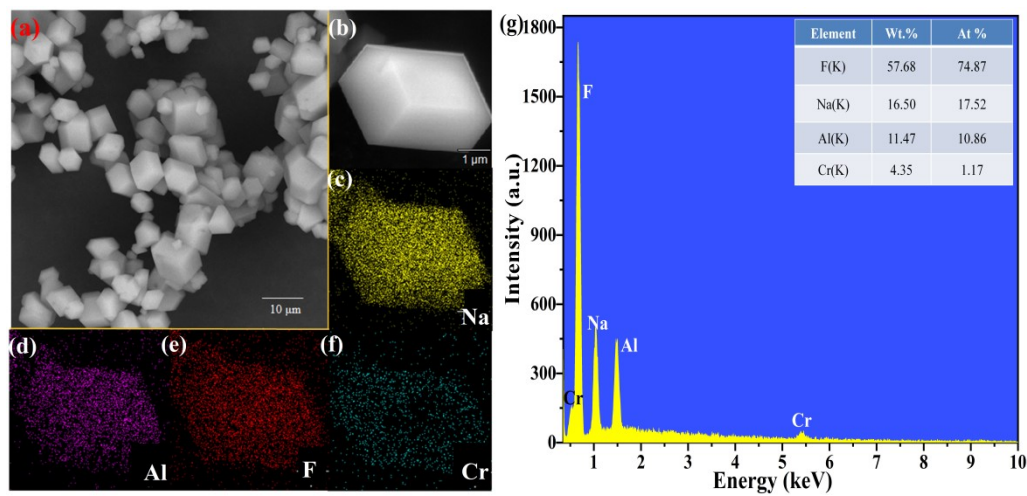
S2 Rietveld refinements of NGaLF:0.16Cr³⁺ (a), NGaLF:0.24Cr³⁺ (b) and NGaLF:0.32Cr³⁺ (c).



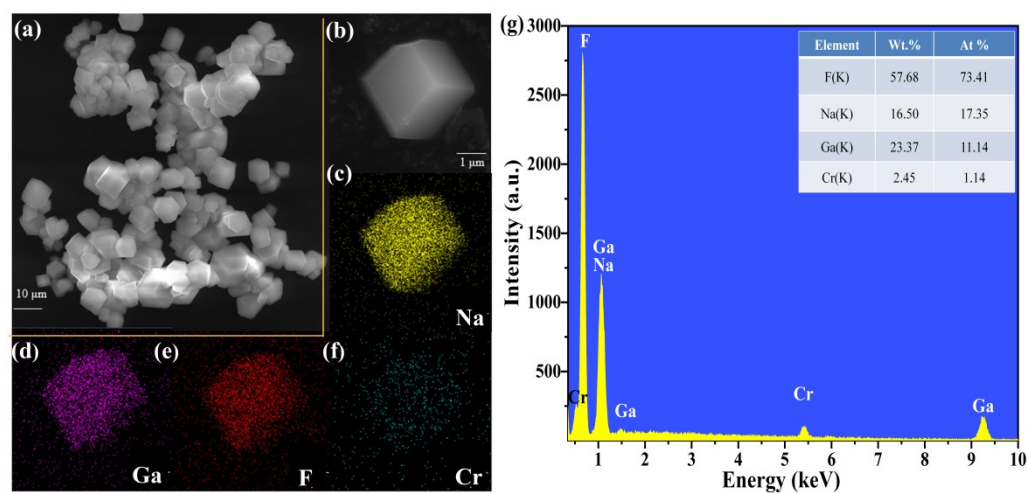
S3 Rietveld refinements of NInLF:0.16Cr³⁺ (a), NInLF:0.24Cr³⁺ (b) and NInLF:0.32Cr³⁺ (c).



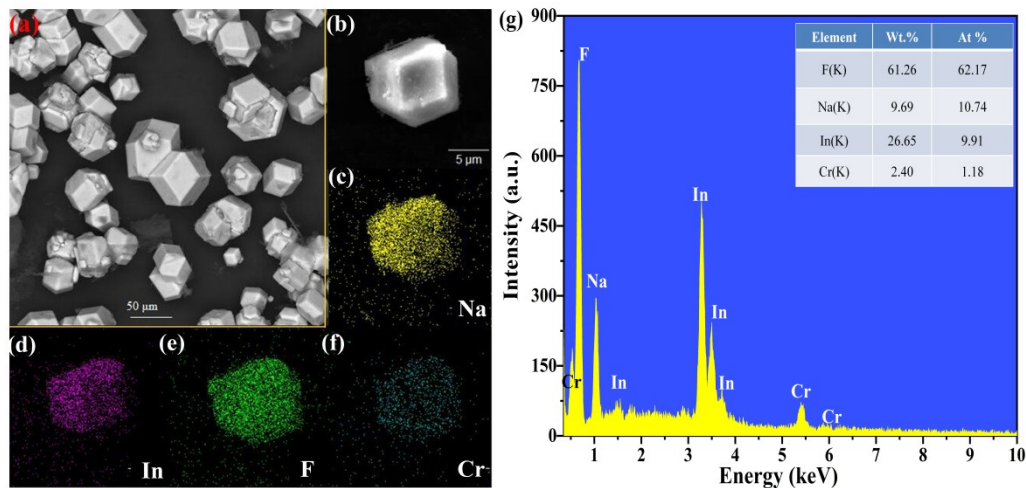
S4 (a,b) Changes of X-F bond length and crystal parameter $a=b=c$ of $NXLF: xCr^{3+}$ ($X=Al, Ga, In$)



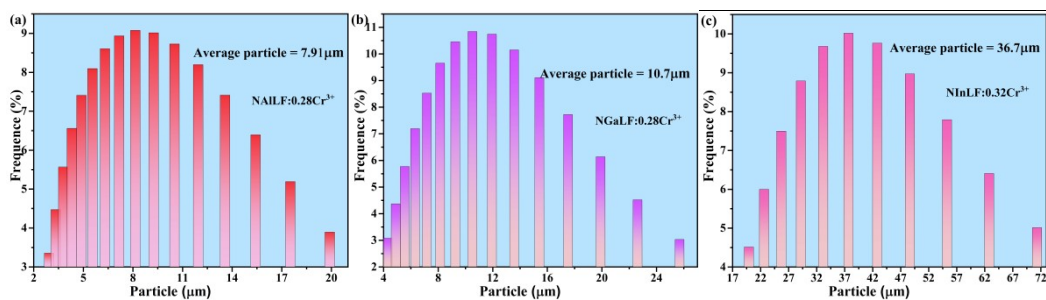
S5 (a,b) the SEM images of $NAlF_3: 0.28Cr^{3+}$ samples. (c-f) elemental mapping of a $NAlF_3: 0.28Cr^{3+}$ single particle, and the corresponding EDS spectrum (g).



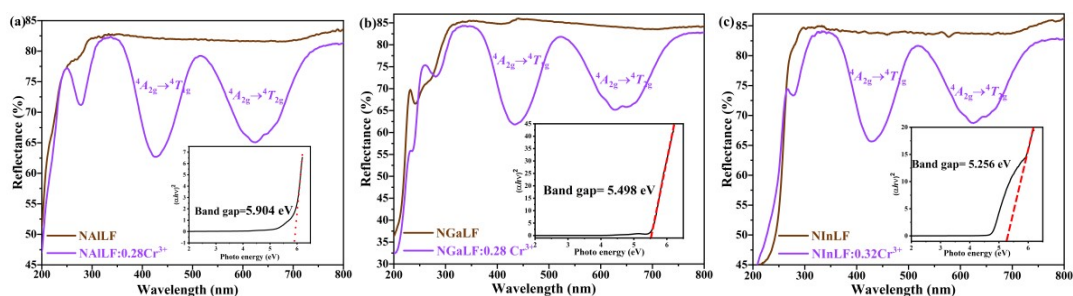
S6 (a,b) the SEM images of $NGaF_3: 0.28Cr^{3+}$ samples. (c-f) elemental mapping of a $NGaF_3: 0.28Cr^{3+}$ single particle, and the corresponding EDS spectrum (g).



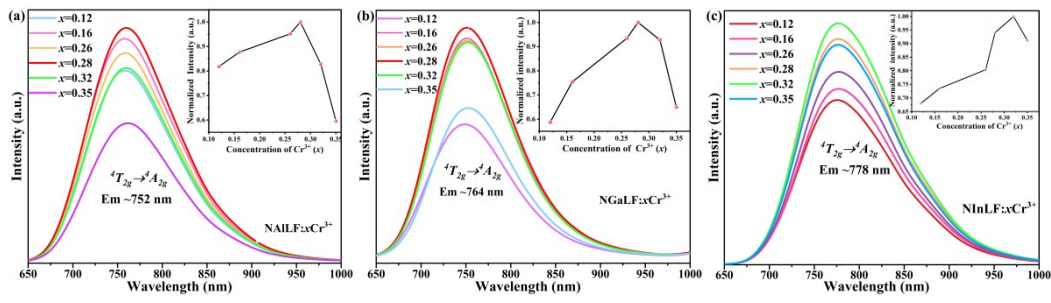
S7 (a,b) the SEM images of NiInLF: 0.28Cr^{3+} samples. (c-f) elemental mapping of a NiInLF: 0.28Cr^{3+} single particle, and the corresponding EDS spectrum (g).



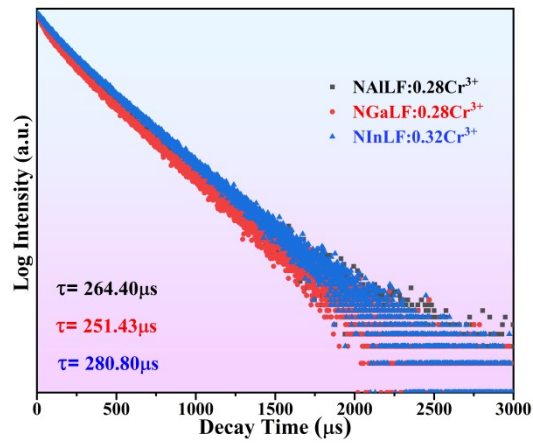
S8 Particle size distribution of NiAlLF: 0.28Cr^{3+} (a), NiGaLF: 0.28Cr^{3+} (b) and NiInLF: 0.28Cr^{3+} (c).



S9 (a) The DRS spectra of NiAlLF and NiAlLF: 0.28Cr^{3+} , (b) The DRS spectra of NiGaLF and NiGaLF: 0.28Cr^{3+} , (c) The DRS spectra of NiInLF and NiInLF: 0.32Cr^{3+} (the insets represent the relationship of $(h\nu)^2$ vs $h\nu$ of NiXLF (X=Al, Ga, In))



S10 The PL spectra of NAILF: $x\text{Cr}^{3+}$ (a), NGalF: 0.28Cr^{3+} (b) and NInLF: 0.32Cr^{3+} (c)



S11 The decay curves of Cr^{3+} in NXLF: $x\text{Cr}^{3+}$ ($X=\text{Al}, \text{Ga}, \text{In}$)

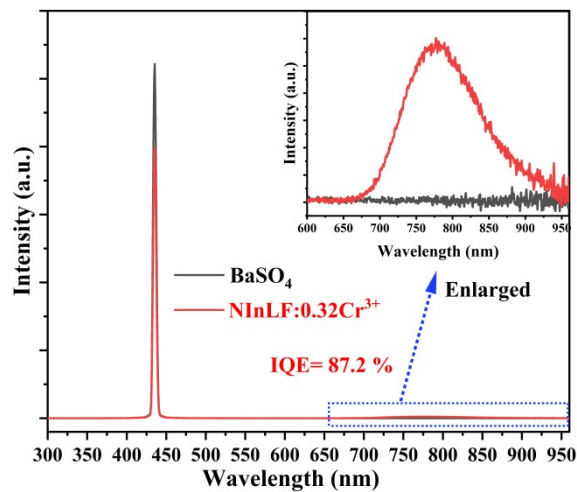
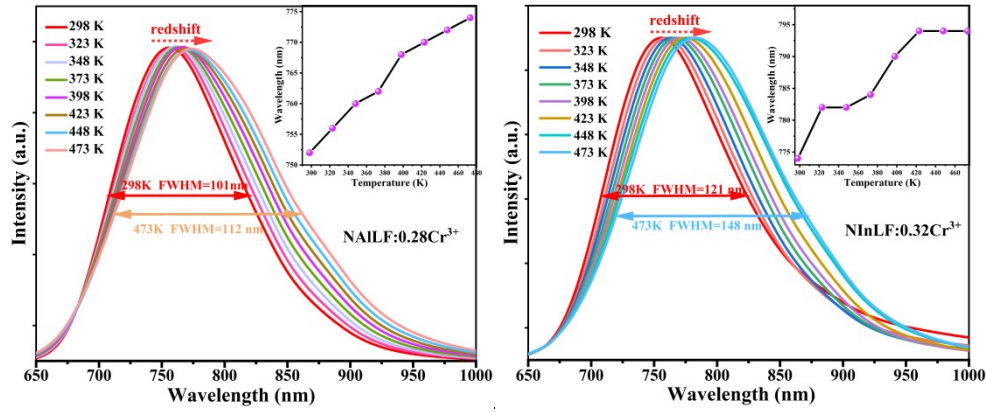
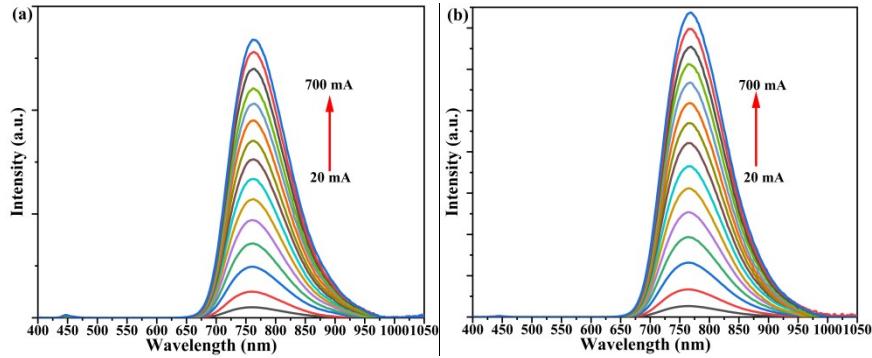


Fig. S12 Emission spectrum of NInLF: 0.32Cr^{3+} phosphor measured using an integrating sphere.



S13 Temperature-dependent PL spectra of NAILF:0.28Cr³⁺ (a) and NInLF:0.28Cr³⁺ (b), the insets represent the changes of emission peak position with increasing temperature.



S14 Electroluminescence spectra of NIR-pc-LED on basis of NAILF:0.28Cr³⁺(a), and NInLF:0.28Cr³⁺(b).

Table S1 Refinement parameters of NAILF: xCr³⁺ phosphors

Formula	x=0	x=0.08	x=0.16	x=0.24	x=0.32
Space group	I a -3 d	I a -3 d	I a -3 d	I a -3 d	I a -3 d
Crystal system	Cubic	Cubic	Cubic	Cubic	Cubic
a=b=c (Å)	12.102	12.14284	12.15449	12.16520	12.17897
$\alpha = \beta = \gamma (^{\circ})$	90	90	90	90	90
Z	8	8	8	8	8
Volume(Å ³)	1771.5	1790.459	1795.607	1800.3513	1806.475
R _p (%)	-	6.03	4.99	4.51	6.02
R _{wp} (%)	-	7.90	6.33	5.74	5.58
χ^2	-	3.719	2.428	3.466	3.945

Al-F length (Å)	1.8113	1.818435	1.822302	1.82792(4)	1.830420
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Table S2 Refinement parameters of NGalF: $x\text{Cr}^{3+}$ phosphors

Formula	$x=0$	$x=0.08$	$x=0.16$	$x=0.24$	$x=0.32$
Space group	I a -3 d	I a -3 d	I a -3 d	I a -3 d	I a -3 d
Crystal system	Cubic	Cubic	Cubic	Cubic	Cubic
a=b=c (Å)	12.312	12.30827	12.311298	12.31	12.313
$\alpha = \beta = \gamma (^{\circ})$	90	90	90	90	90
Z	8	8	8	8	8
Volume(Å³)	1865.4	1864.621	1866.000	1865.40979	1866.9123
R_p(%)	-	7.97	7.25	7.06	7.26
R_{wp}(%)	-	9.28	9.71	9.69	9.94
χ^2	-	1.309	1.120	1.122	1.182
Ga-F length (Å)	1.8843	1.886513	1.887540	1.885570	1.894121

Table S3 Refinement parameters of NInLF: $x\text{Cr}^{3+}$ phosphors

Formula	$x=0$	$x=0.08$	$x=0.16$	$x=0.24$	$x=0.32$
Space group	I a -3 d	I a -3 d	I a -3 d	I a -3 d	I a -3 d
Crystal system	Cubic	Cubic	Cubic	Cubic	Cubic
a=b=c (Å)	12.69431	12.6875	12.67916	12.67086	12.66046
$\alpha = \beta = \gamma (^{\circ})$	90	90	90	90	90
Z	8	8	8	8	8
Volume(Å³)	2045.63	2042.3614	2038.318	2034.319	2029.319
R_p(%)	-	7.06	8.686	8.71	8.67
R_{wp}(%)	-	5.44	5.83	6.16	5.89
χ^2	-	3.898	4.876	4.555	4.556
In-F length (Å)	2.063718	2.02459(4)	1.99385(2)	1.98193(6)	1.961936

Table S4 Refinement parameters of N_{Ga}LF: 0.28Cr³⁺ phosphor at different temperatures.

Formula	298K	323K	373K	423K
Space group	I a -3 d	I a -3 d	I a -3 d	I a -3 d
Crystal system	Cubic	Cubic	Cubic	Cubic
a=b=c (Å)	12.31	12.33	12.35	12.37
$\alpha = \beta = \gamma (^{\circ})$	90	90	90	90
Z	8	8	8	8
Volume(Å³)	1865.40	1875.10	1885.56	1895.30
R_p(%)	9.98	9.81	10.22	10.40
R_{wp}(%)	7.41	7.18	7.51	7.59
χ^2	3.225	3.118	3.366	3.493
Ga-F length (Å)	1.856678	1.858361	1.861412	1.862724