

Supporting Information

Broadband short-wave near-infrared-emitting phosphor

MgNb₂O₆:Cr³⁺ for *pc*-LED applications

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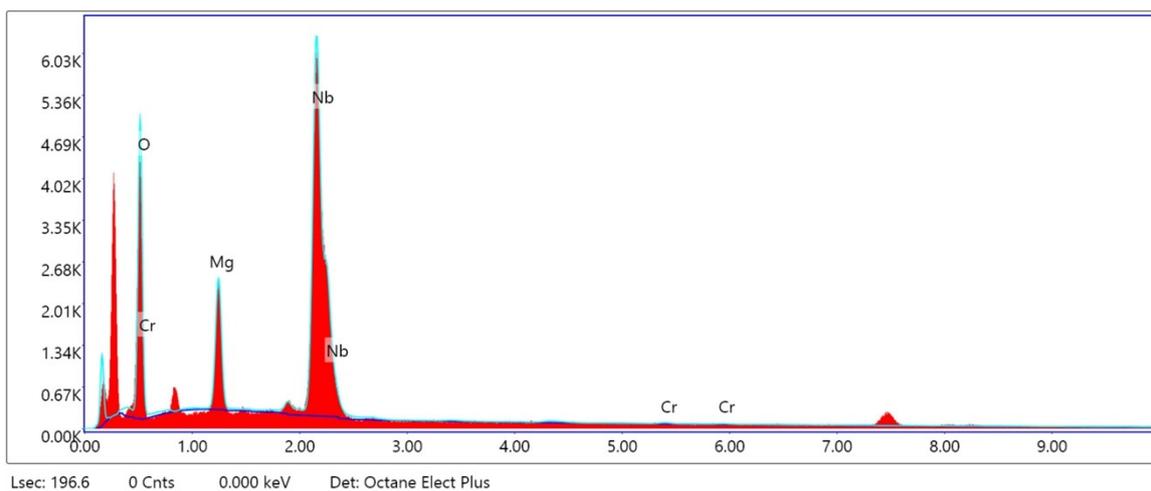


Figure S1 The EDS analysis spectra of the $\text{MgNb}_2\text{O}_6:1\%\text{Cr}^{3+}$ phosphor

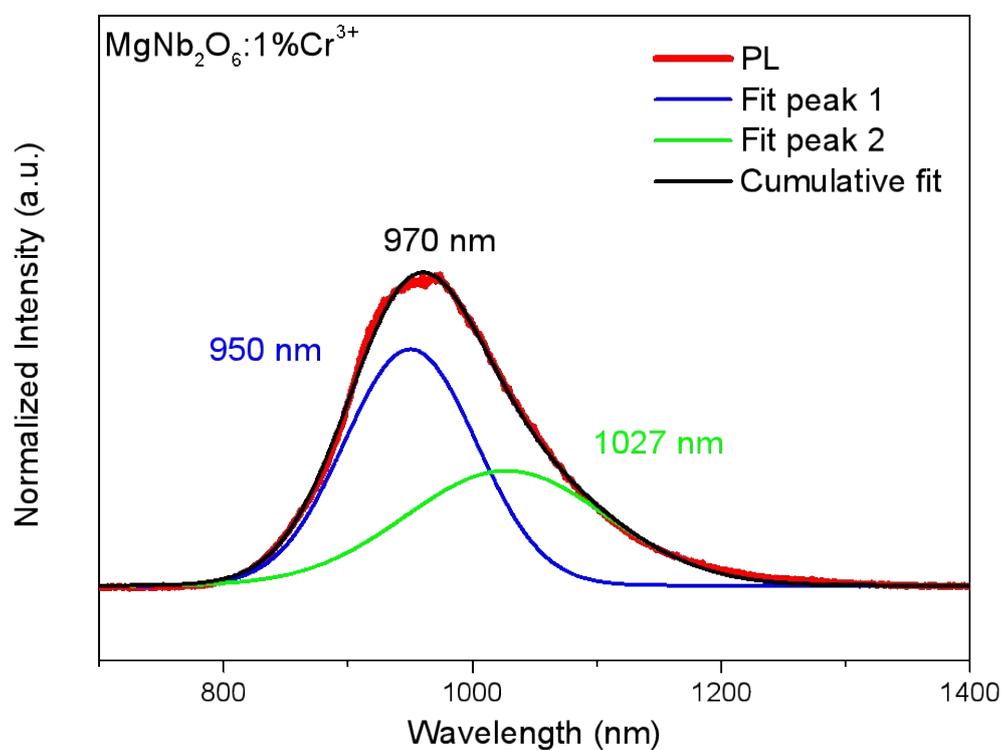


Figure S2 A Gaussian fitting for the PL spectrum of the $\text{MgNb}_2\text{O}_6:1\%\text{Cr}^{3+}$ phosphor

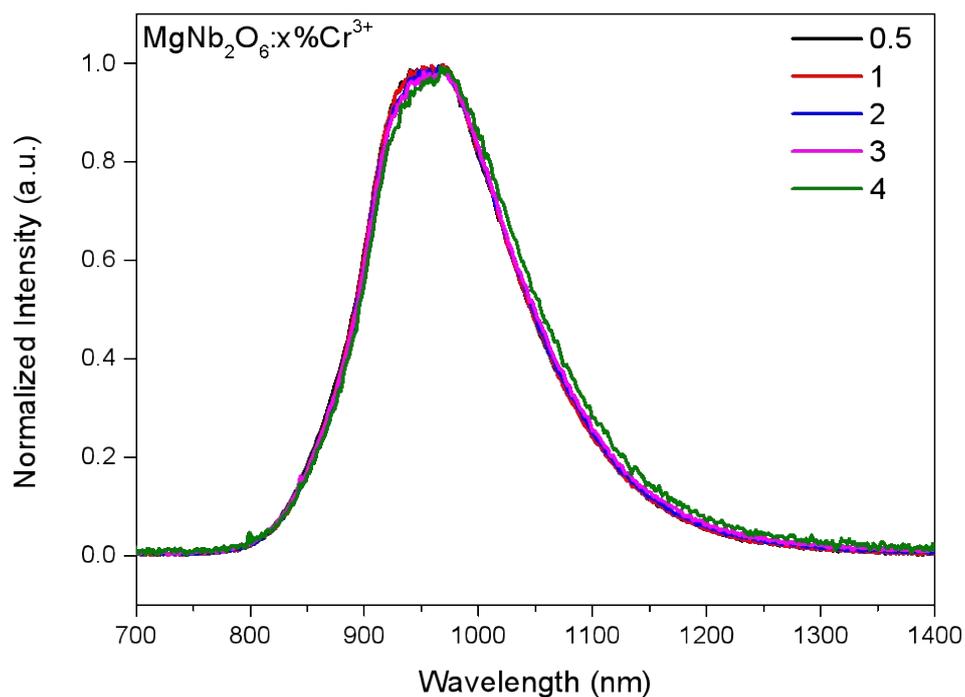


Figure S3 Normalized PL spectra of the $\text{MgNb}_2\text{O}_6:x\%\text{Cr}^{3+}$ ($x = 0.5, 1, 2, 3, 4$) samples under excitation of 515 nm.

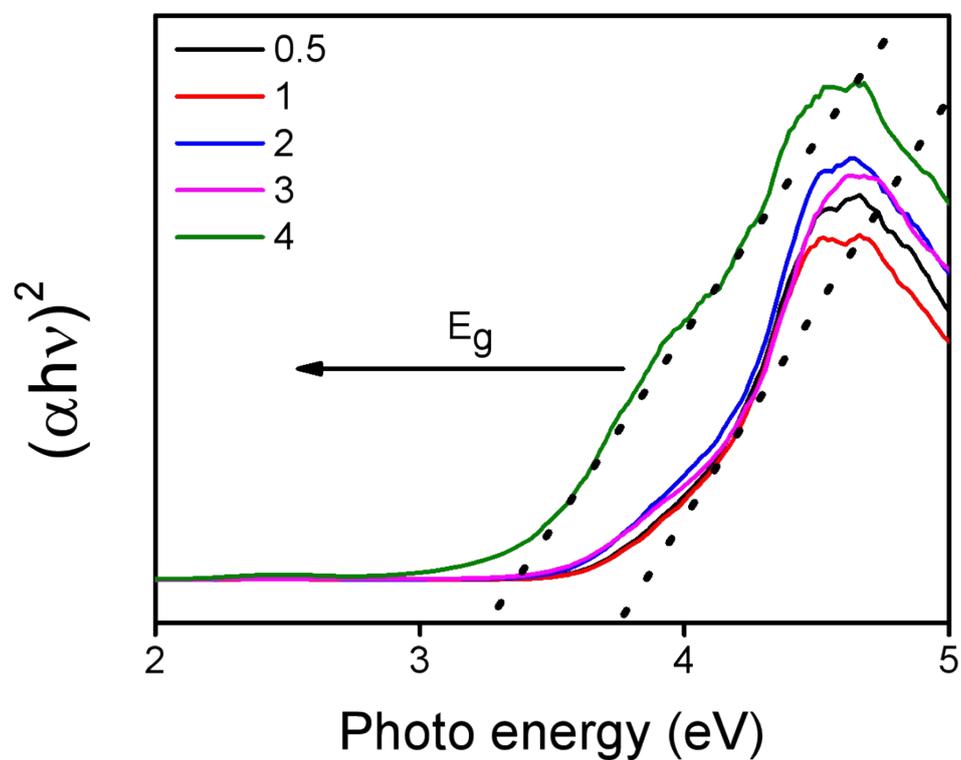


Figure S4 The calculated bandgap (E_g) of the $\text{MgNb}_2\text{O}_6:x\%\text{Cr}^{3+}$ ($x = 0.5, 1, 2, 3, 4$) phosphor samples.

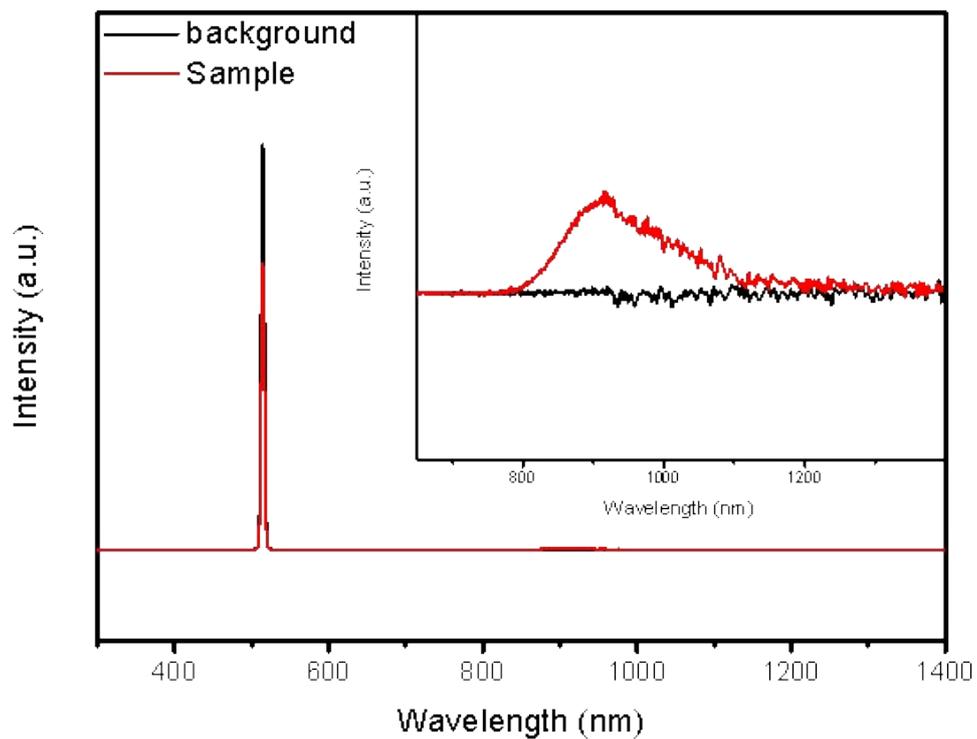


Figure S5 The measured spectra for determining the photoluminescence quantum yield of the $\text{MgNb}_2\text{O}_6:1\%\text{Cr}^{3+}$ sample.

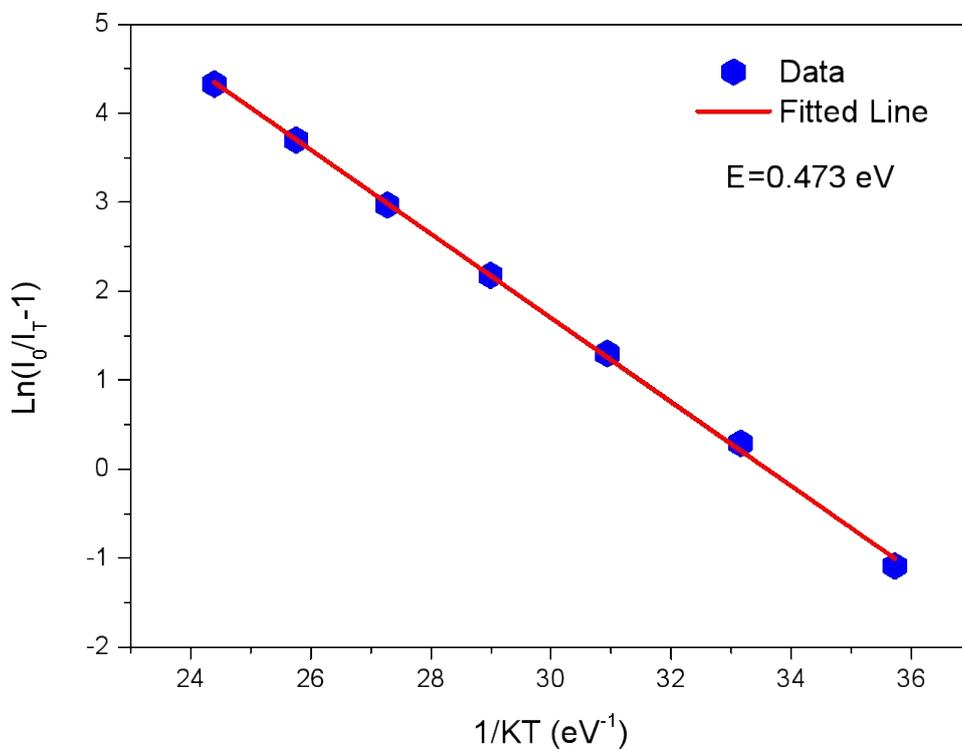


Figure S6 $\ln(I_0/I_T - 1)$ versus $1/KT$ plot of the temperature dependent spectra ($I_0 = I_{298\text{K}}$)

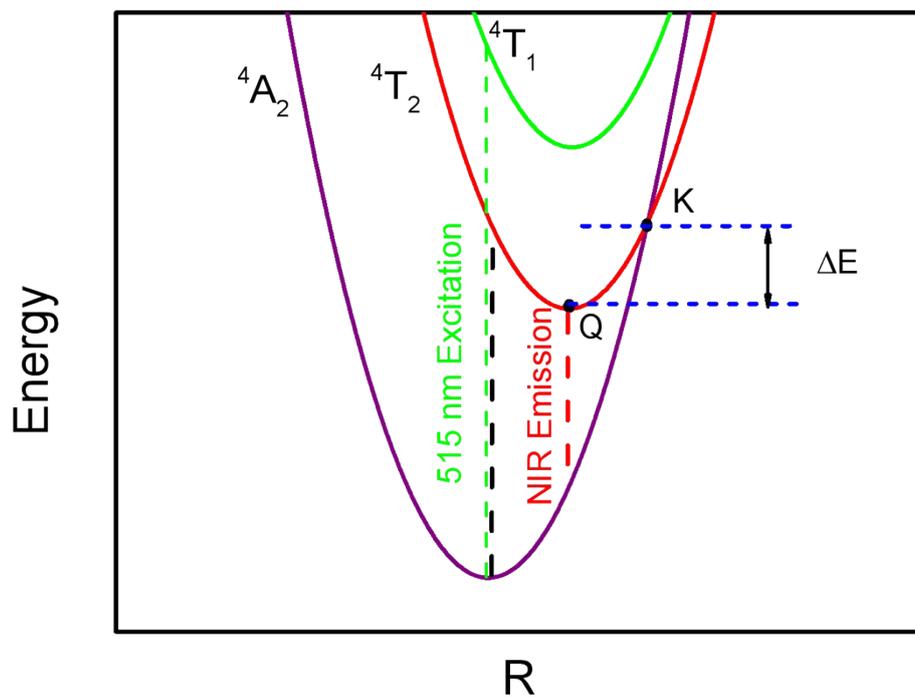


Figure S7 Configurational coordinate diagram of thermal quenching behavior for the $\text{MgNb}_2\text{O}_6:1\%\text{Cr}^{3+}$ optimal sample

Table S1 The crystal parameters of the MgNb₂O₆ host

Compound	MgNb ₂ O ₆	Bond	value
Space group	P b c n (60)	Mg-O1	2.081 Å
a	14.1875 Å	Mg-O2	2.081 Å
b	5.7001 Å	Mg-O3	2.082 Å
c	5.0331 Å	Mg-O4	2.082 Å
a/b	2.4890	Mg-O5	2.132 Å
b/c	1.1325	Mg-O6	2.132 Å
c/a	0.3548	Nb-O1	2.080 Å
V	407.03(1) Å ³	Nb-O2	1.910 Å
Z	4	Nb-O3	1.795 Å
		Nb-O4	2.071 Å
Average Mg-O	Average Nb-O	Nb-O5	1.960 Å
2.065 Å	2.014 Å	Nb-O6	2.272 Å

Table S2 Calculated crystal lattice parameters of the as-prepared MgNb₂O₆:x%Cr³⁺ (x = 0, 0.5, 1, 2, 3, 4) phosphor samples

Samples	a	b	c	V
x = 0	14.1875 Å	5.7001 Å	5.0331 Å	407.030 Å ³
x = 0.5	14.1875 Å	5.6989 Å	5.0338 Å	407.012 Å ³
x = 1	14.1891 Å	5.6995 Å	5.0325 Å	406.994 Å ³
x = 2	14.1858 Å	5.7001 Å	5.0332 Å	406.991 Å ³
x = 3	14.1892 Å	5.6995 Å	5.0325 Å	406.719 Å ³
x = 4	14.1839 Å	5.6984 Å	5.0314 Å	406.668 Å ³

Table S3 Results of EDS mapping of the MgNb₂O₆:1%Cr³⁺ representative

Element	Weight %	Atomic %	Net Int.	Error %	K ratio	Z	A	F
Mg	7.66	12.33	148.60	4.56	0.0620	1.0408	0.7726	1.0066
Nb	67.87	28.58	545.20	2.08	0.5469	0.7833	1.0290	0.9997
O	24.03	58.75	238.30	8.29	0.0982	1.1200	0.3648	1.0000
Cr	0.44	0.33	2.20	59.15	0.0040	0.9055	0.9764	1.0244

Table S4 Fitting functions, R-square, and calculated decay time of the MgNb₂O₆:x%Cr³⁺ (x = 0.5, 1, 2, 3, 4) monitoring at 970 nm under pulsed light excitation of 515 nm

Sample	fitting function	τ_1 (μ s)	τ_2 (μ s)	τ_{avg} (μ s)	R-square
MgNb ₂ O ₆ :0.5%Cr ³⁺	$I = A_1 * \exp(-t/\tau_1) + A_2 * \exp(-t/\tau_2) + I_0$	10.29	10.29	10.29	0.99898
MgNb ₂ O ₆ :1%Cr ³⁺	$I = A_1 * \exp(-t/\tau_1) + A_2 * \exp(-t/\tau_2) + I_0$	10.20	10.20	10.20	0.99911
MgNb ₂ O ₆ :2%Cr ³⁺	$I = A_1 * \exp(-t/\tau_1) + A_2 * \exp(-t/\tau_2) + I_0$	9.43	9.43	9.43	0.99917
MgNb ₂ O ₆ :3%Cr ³⁺	$I = A_1 * \exp(-t/\tau_1) + A_2 * \exp(-t/\tau_2) + I_0$	7.13	13.5	8.19	0.9993
MgNb ₂ O ₆ :4%Cr ³⁺	$I = A_1 * \exp(-t/\tau_1) + A_2 * \exp(-t/\tau_2) + I_0$	11.00	3.91	5.09	0.99905

Table S5 The NIR output power and photoelectric efficiency of MgNb₂O₆:1%Cr³⁺ pc-LED and that of some reported similar pc-LED devices

Phosphors	Chip (nm)	Peak (nm)	NIR output power	Photoelectric efficiency	Ref
NaInGe ₂ O ₆ :7%Cr ³⁺	470	900	25.2 mW@ 120 mA	8.2%@20 mA	S1
Mg ₃ Ga _{1.9} In _{0.1} GeO ₈ :3%Cr ³⁺	455	910	6.134 mW@ 60 mA	8.5%@60 mA	S2
ZnTa ₂ O ₆ :4%Cr ³⁺	460	935	39.8 mW@ 300 mA	5%@100 mA	S3
Li ₃ Sc ₂ (PO ₄) ₃ :8%Cr ³⁺	496	978	5.81 mW@ 80mA	2.62%@80 mA	S4
MgNb ₂ O ₆ :1%Cr ³⁺	515	970	6.29 mW@ 100mA	2.5%@100 mA	This work

Reference

- S1. W. Zhou, J. Luo, J. Fan, H. Pan, S. Zeng, L. Zhou, Q. Pang and X. Zhang, *Ceram. Int.*, 2021, **47**, 25343-25349.
- S2. D. Dai, Z. Wang, Z. Xing, X. Li, C. Liu, L. Zhang, Z. Yang and P. Li, *J. Alloys Compd.*, 2019, **806**, 926-938.
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- S4. S. Zhao, L. Lou, S. Yuan, D. Zhu, F. Wu and Z. Mu, *J. Lumin.*, 2022, **251**, 119188.