Supplementary information

A novel near-infrared phosphor $Li_{1.6}Mg_{1.6}Sn_{2.8}O_8$:$Cr^{3+}$ for near-infrared spectral analysis

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Tables and Table Captions

Table S1 Refined structural data of $Li_{1.6}Mg_{1.6-0.5x}Sn_{2.8-0.5x}O_8$: xCr^{3+} (x = 0 and 0.06) samples

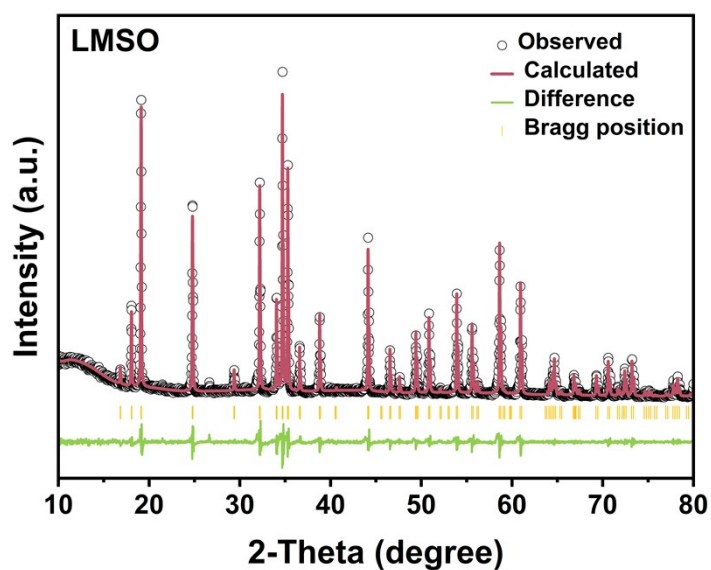| Samples	Cell parameters			Volume (Å³)	R_{wp}, R_p, %, χ^2
(x)	a (Å)	b (Å)	c (Å)		
0	6.07990	6.07990	9.81940	314.35	10.10, 8.27, 2.638
0.06	6.06612	6.06612	9.80590	312.49	9.33, 7.04, 2.030

Table S2 The atom positions, fraction factors, and thermal vibration parameters of $Li_{1.6}Mg_{1.6-0.5x}Sn_{2.8-0.5x}O_8$: xCr^{3+} (x = 0 and 0.06) samples.

			$Li_{1.6}Mg_{1.6}Sn_{2.8}O_8$			
Atom	x	y	z	Occpancy	U_{iso}	Mutl
Sn1	0.3333	0.6667	-0.23042	1.0	0.00515	2
Sn2	0.16695	-0.16695	-0.50788	0.6	0.00449	6
Mg2	0.16695	-0.16695	-0.50788	0.2	0.00938	6
Li2	0.16695	-0.16695	-0.50788	0.2	0.00938	6
Mg1	0.3333	0.6667	-0.81859	1.0	0.06385	2
Li1	0.0	0.0	-0.24695	1.0	0.21204	2
O1	0.0	0.0	-0.3902	1.0	-0.01616	2
O2	0.3333	0.6667	-0.62466	1.0	0.02986	2
O3	0.49011	-0.49011	-0.37331	1.0	0.01334	6
O4	0.15724	-0.15724	-0.12332	1.0	0.00689	6

			$Li_{1.6}Mg_{1.6}Sn_{2.8}O_8$:$0.06Cr^{3+}$			
Atom	x	y	z	Occpancy	U_{iso}	Mutl
Sn1	0.3333	0.6667	0.49893	0.985	0.00762	2
Sn2	0.16695	-0.16695	0.21963	0.5925	0.00986	6
Mg2	0.16695	-0.16695	0.21963	0.1925	0.02132	6
Li2	0.16695	-0.16695	0.21963	0.2	0.02132	6
Mg1	0.3333	0.6667	-0.0845	1.0	0.09415	2
Li1	0.0	0.0	0.46639	1.0	0.07077	2
O1	0.0	0.0	0.325	1.0	-0.00988	2
O2	0.3333	0.6667	0.10661	1.0	-0.04027	2
O3	0.48988	-0.48988	0.35794	1.0	0.01773	6
O4	-0.15715	-0.15715	0.59815	1.0	0.04301	6
Cr1	0.3333	0.6667	0.49893	0.015	0.02249	2
Cr2	0.16808	-0.16808	0.21963	0.015	0.02859	6

Table S3 Parameters of crystal field theory at different Concentration

Concentration (x)	$^4A_2 \rightarrow {}^4T_1$ (cm^{-1})	$^4A_2 \rightarrow {}^4T_2$ (cm^{-1})	$^4T_2 \rightarrow {}^4A_2$ (cm^{-1})	ΔS	Dq	Dq/B
0.02	23111.77	16109.54	11737.09	4372.45	1392.33	1.78
0.04	23116.58	16156.92	11668.61	4488.31	1391.28	1.78
0.06	23169.60	16145.18	11627.91	4517.27	1388.65	1.77
0.08	23180.34	16145.96	11520.74	4625.22	1383.33	1.75
0.10	23191.09	16143.35	11428.57	4714.78	1378.6	1.73
0.12	23234.67	16200.09	11397.65	4802.44	1378.52	1.72
0.15	23348.12	16243	11325.03	4917.97	1378.4	1.71

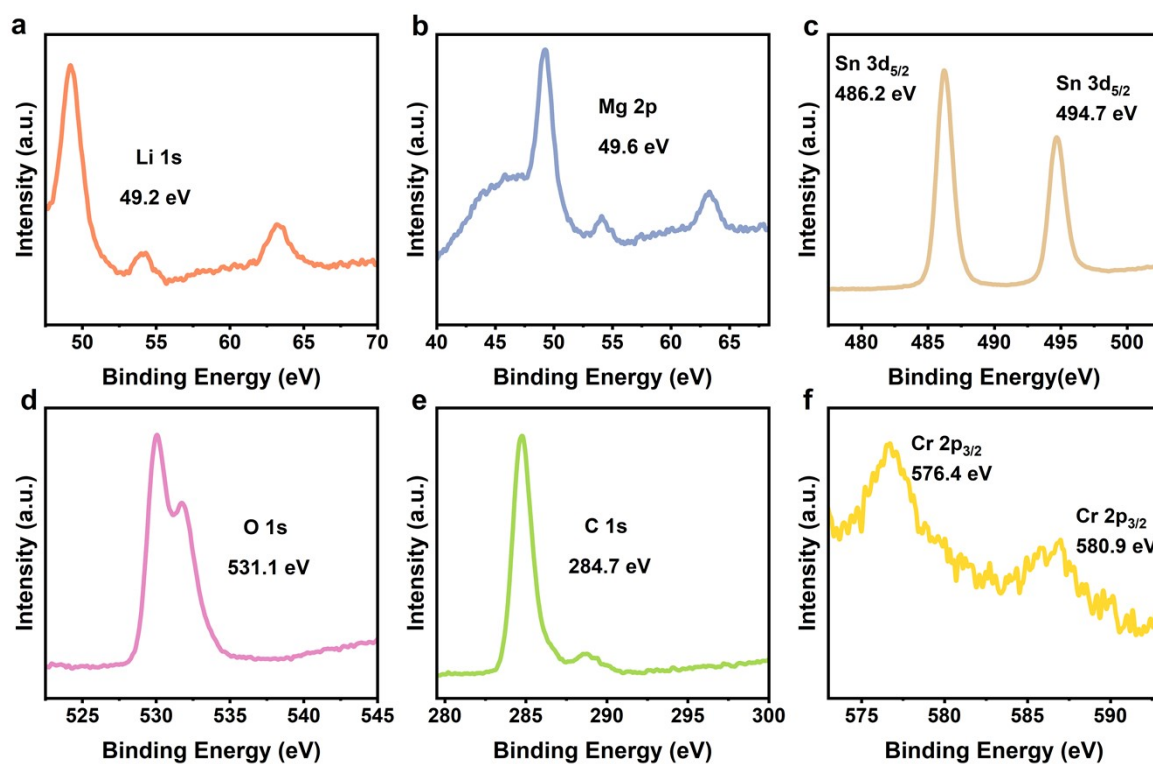**Figure S1** Rietveld refinement of LMSO.

Figure S2 XPS spectrogram of the LMSO:Cr^{3+} phosphors. (a) Li-1s, (b) Mg-2p, (c) Sn-3d, (d) O-1s, (e) C-1s and (f) Cr-2p.
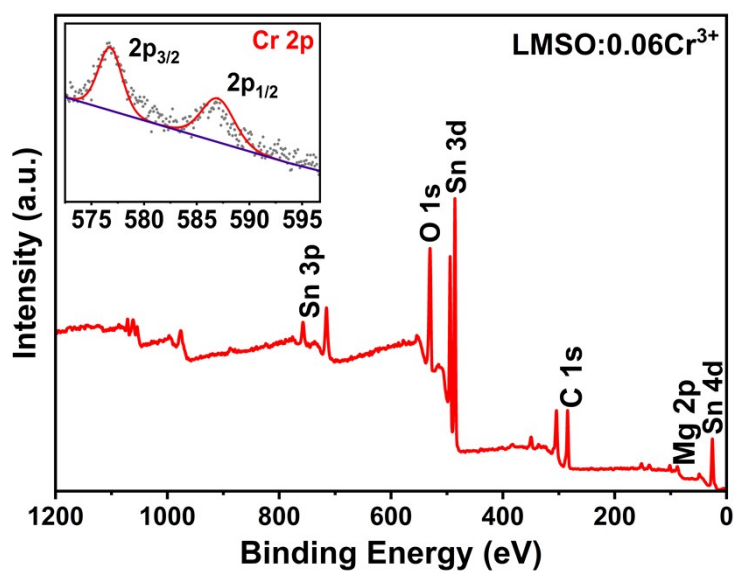

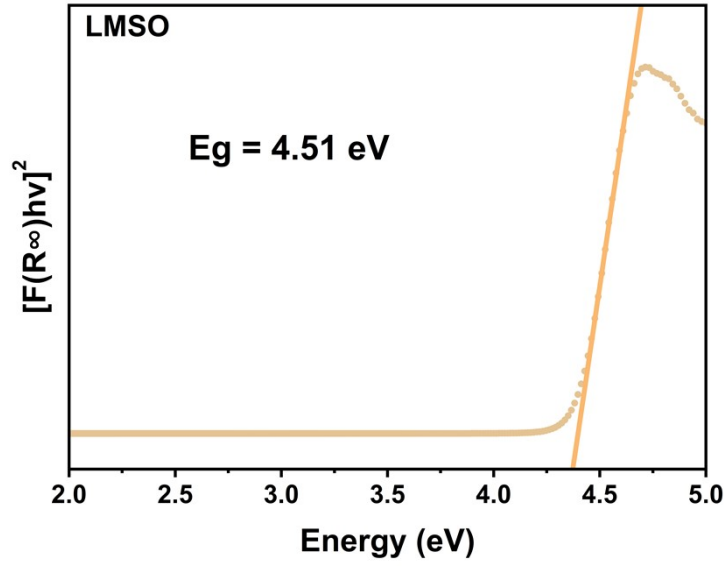**Figure S3** High-resolution Cr 2p XPS core energy level spectra of LMSO:0.06Cr^{3+}.

Figure S4 The absorption spectrum of LSMO calculated using the Kubelka–Munk equation.

The optical bandgap of the samples can be calculated by the Kubelka-Munk function as follows[1]：

$$F(R) = (1-R)^2 / 2R \qquad (1)$$

$$(F(R) \times hv) = A(hv - Eg) \qquad (2)$$

where hv is the optical energy, A is a constant, E_g is the direct bandgap, α is the absorption coefficient, R is the reflectance in the DR spectrum, n is the transition coefficient and R_∞ is the reflectance of the infinitely thick sample for each wavelength reference point. The calculated of the LMSO is 4.51 eV as shown in the inset of Figure S4.
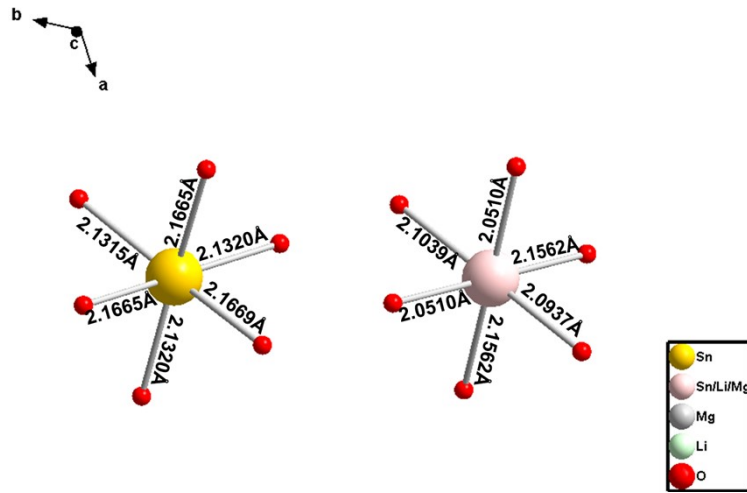
Figure S5 Structural diagram of LMSO crystal.

Calculation of the crystal field

Broadband NIR emission spectra were observed in LMSO:Cr^{3+}, suggesting that the Cr^{3+} ion is located in a relatively weak crystal field. The crystal field strength Dq/B can be calculated using the following formula[2]:

$$\Delta E = E(^4A_2 - {}^4T_1) - (^4A_2 - {}^4T_2) \tag{3}$$

$$\Delta S = E(^4A_2 - {}^4T_2) - (^4T_2 - {}^4A_2) \tag{4}$$

$$10Dq = E(^4T_2) = E(^4A_2 - {}^4T_2) - \Delta S \tag{5}$$

$$\frac{Dq}{B} = \frac{15(^4\Delta E / Dq - 8)}{(\Delta E / Dq)^2 - 10(\Delta E / Dq)} \tag{6}$$

In the equation, Dq represents the crystal field parameter, B represents the Racah parameter, ΔE represents the energy difference between the $^4T_1$ and $^4T_2$ energy levels, The values of $E(^4T_2)$ and $E(^4T_1)$ are calculated from the energy positions corresponding to the excitation bands. It is worth noting that when there is a Stokes shift, the energy position $E(^4T_2)$ is not strictly equal to the transition energy $E(^4A_2 \rightarrow {}^4T_2)$, and the effect of the Stokes shift (ΔS) needs to be considered. The energy difference between $^4A_2 \rightarrow {}^4T_2$ and $^4T_2 \rightarrow {}^4A_2$ is used to compute the value of ΔS. The calculated values of Dq and B are approximately 1388.65 and 784.54 cm^{-1}, respectively.
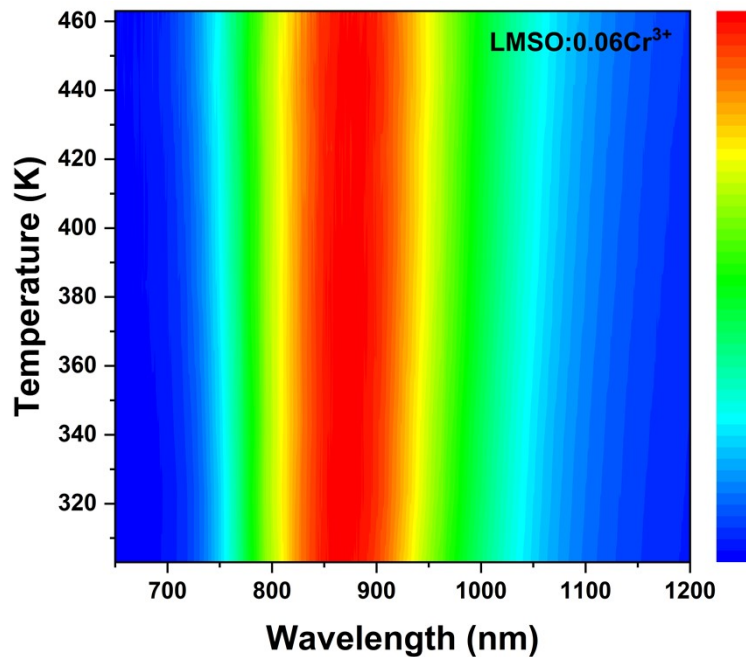
Figure S6 Normalized emission intensity variable temperature mapping image of LMSO:0.06Cr³⁺.

The IQE of LMSO:0.06Cr³⁺

Quantum efficiency is an important parameter for evaluating the luminescence performance of phosphors. However, directly measuring the quantum efficiency of near-infrared phosphors excited by blue light is quite challenging. Therefore, we adopted a segmented method to measure the quantum yield of LMSO:0.06Cr³⁺ phosphor and carefully calibrated the sensitivity of the two-step test.

[1] J. Zhou, Z. Long, J. Qiu, D. Zhou, Y. Yang, K. Zhang, W. Shen, Q. Wang, Broadband near-infrared emitting from $Li_{1.6}Zn_{1.6}Sn_{2.8}O_8$:Cr³⁺ phosphor by two-site occupation and Al³⁺ cationic regulation, Materials & Design, 192 (2020) 108701.

[2] S. Wang, R. Pang, X. Chen, T. Tan, Q. Wang, C. Li, S. Zhang, T. Tan, H. You, H. Zhang, An ultra broadband NIR phosphor $LiScSnO_4$:Cr³⁺ with emission wavelength peaking at 900 nm for component analysis, Ceramics International, 50 (2024) 1452-1460.