Supporting Information

$Ba_3LuGa_2O_{7.5}:Bi^{3+}$ phosphors with potential applications of full-spectrum WLEDs and temperature sensing

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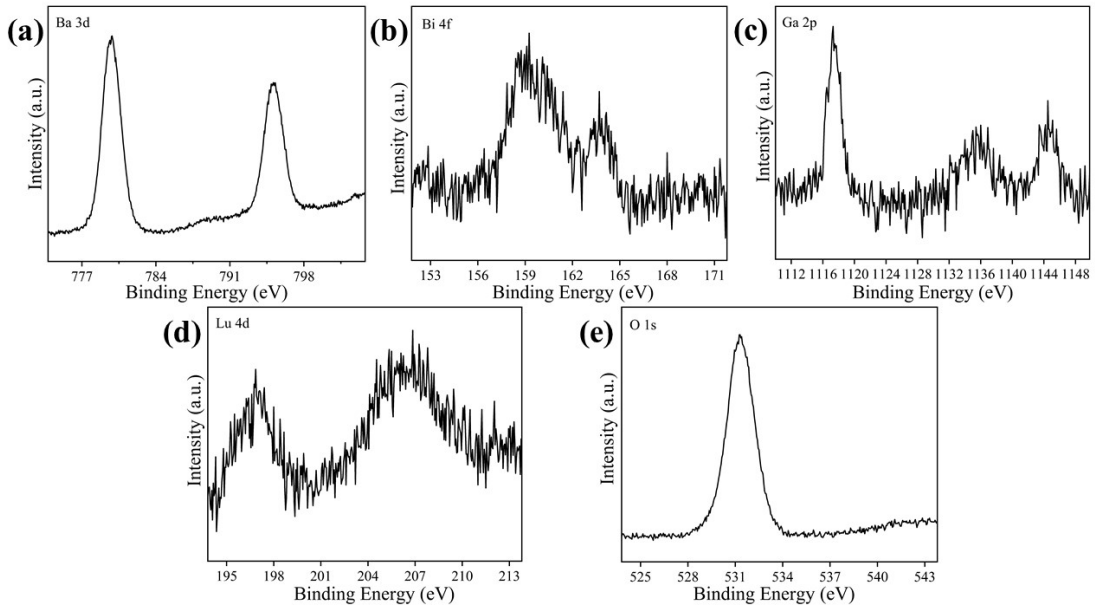

Fig. S1 (a−e) Ba 3d, Bi 4f, Ga 2p, Lu 4d, and O 1s XPS of $Ba_3LuGa_2O_{7.5}$:0.02Bi^{3+} sample.

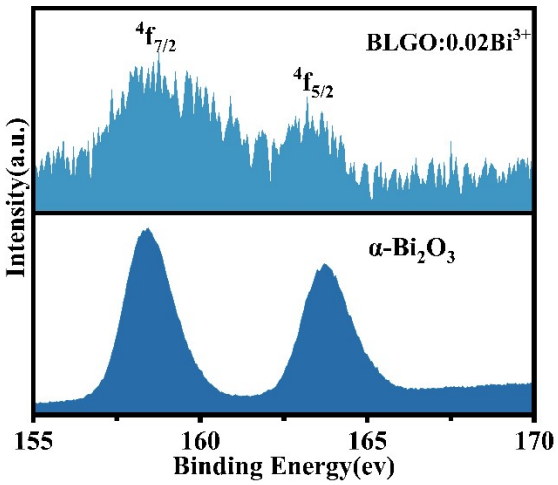

Fig. S2 X-Ray Photoelectron Spectroscopy (XPS) spectra of the $Ba_3LuGa_2O_{7.5}:Bi^{3+}$ sample and α-Bi_2O_3 reference.

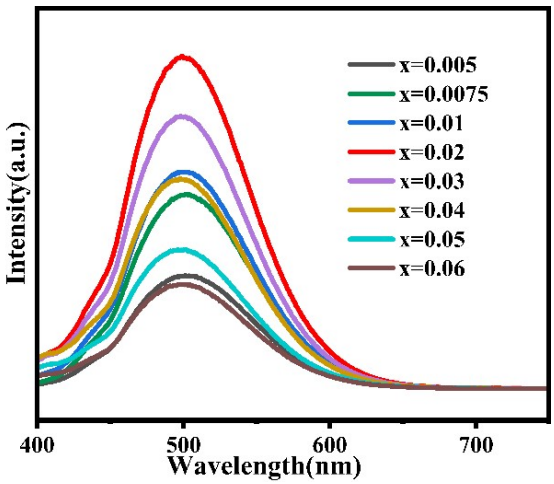

Fig. S3 Emission spectra of $Ba_3LuGa_2O_{7.5}:xBi^{3+}$ under excitation at 351 nm ($0.005 \leq x \leq 0.06$).

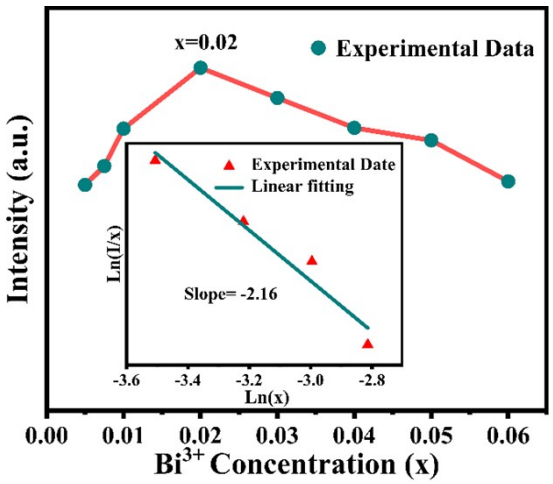

Fig. S4 The dependence of the emission intensity on content of Bi^{3+} ion doping concentration, the inset shows the relationship between Ln(I/x) and Ln(x) for BLGO:xBi^{3+} ($0.005 \leq x \leq 0.06$).

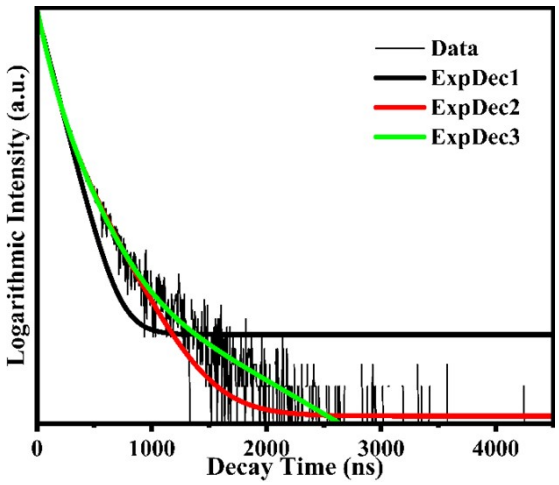

Fig. S5 The three kinds fitting for fluorescence decay curves of BLGO:0.02Bi^{3+}.

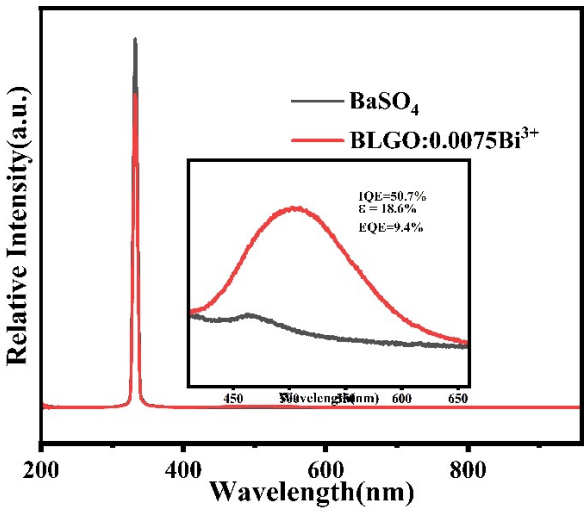

Fig. S6 The QE spectrum of BLGO:0.02Bi^{3+} (the inset is the local enlarged drawing of QE spectrum)

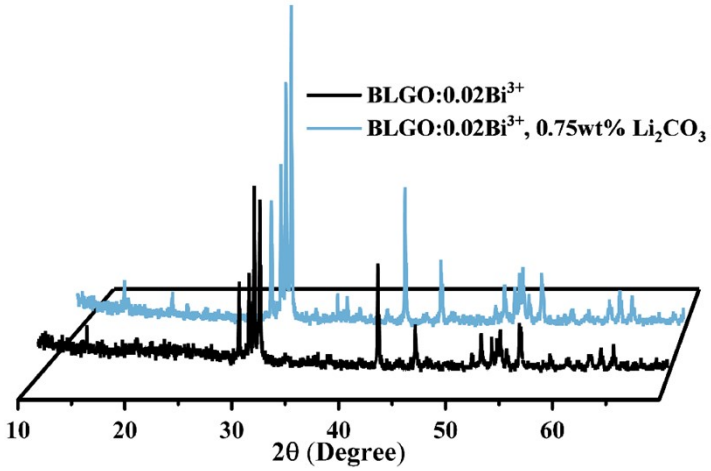

Fig. S7 XRD patterns of BLGO:0.02Bi^{3+} and BLGO:0.02Bi^{3+}, 0.75 wt% Li_2CO_3**.**

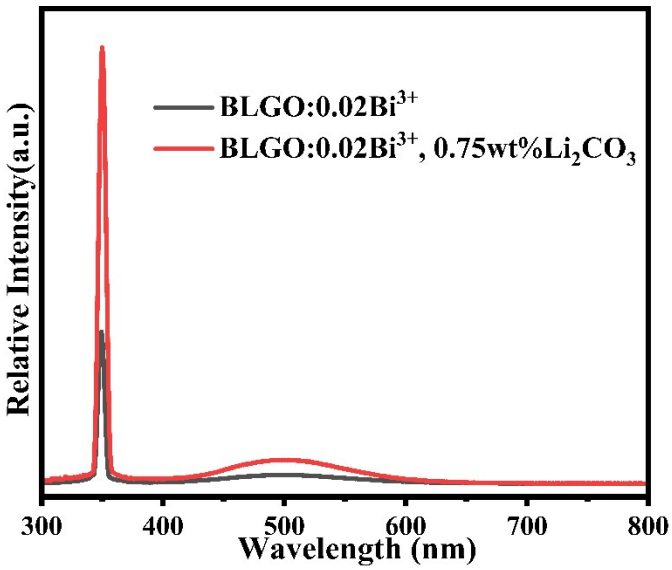

Fig. S8 The QE spectrum of BLGO:0.02Bi^{3+} and BLGO:0.02Bi^{3+}, 0.75 wt % Li_2CO_3.

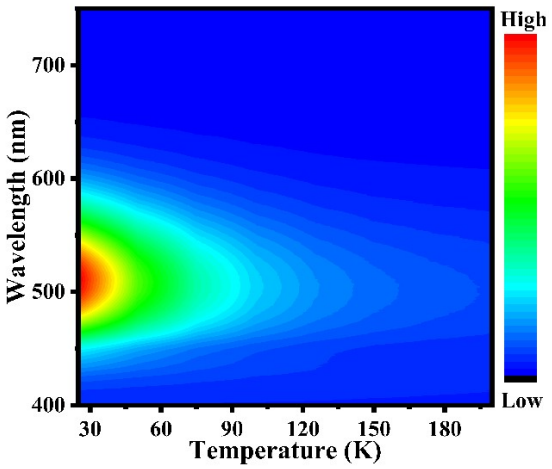

Fig. S9 The contour graph of the thermal quenching behavior of the BLGO:0.02Bi^{3+} sample.

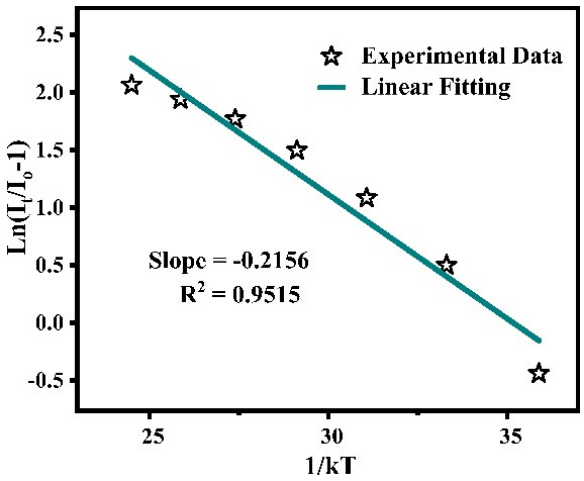

Fig. S10 The relationship of $\ln(I_0/I_T - 1)$ versus $(KT)^{-1}$ for the BLGO:0.02Bi^{3+} phosphor and the fitting curve.

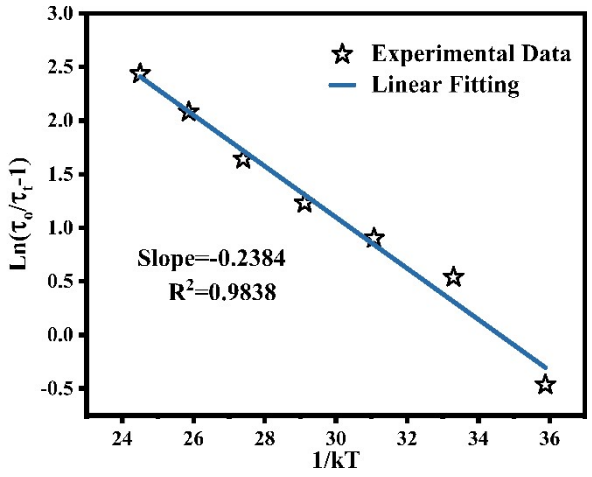

Fig. S11 The relationship of $\ln(\tau_0/\tau_T - 1)$ versus $(KT)^{-1}$ for the BLGO:0.02Bi^{3+} phosphor and the fitting curve.

Table S1 Rietveld fitting results of $Ba_3LuGa_2O_{7.5}$

Formula	BLGO:Bi^{3+}
Crystal system	monoclinic system
Space group	P2/c
a（Å）	18.3941（4）
b（Å）	5.9414（4）
c（Å）	7.9076（2）
α=γ（°）	90.0000(0)
β（°）	91.3802(9)
Z	4
Cell volume（$Å^3$）	863.95(6)
Rp（%）	4.34
Rwp（%）	5.67
Rexp（%）	2.58
χ^2	4.82

Table S2 Atomic positions of $Ba_3LuGa_2O_{7.5}$

Atom	x	y	z	B_{iso}	Occ.
Ba1	0	0.2783(4)	0.25	2.88(8)	0.54(1)
Ba2	0.5	0.3199(9)	0.25	0.86(3)	0.45(4)
Ba3	0.0320(1)	0.7490(8)	0.0899(4)	1.04(0)	0.94(6)
Ba4	0.5062(8)	0.2443(3)	0.5801(4)	0.91(9)	1.05(3)
Lu	0.2487(8)	0.2564(6)	0.4132(4)	0.24(6)	0.97(2)
Ga1	0.2524(9)	0.2529(1)	0.0608(0)	3.27(2)	0.99(1)
Ga2	0.2372(6)	0.7631(7)	0.2697(9)	-0.25(9)	1.02(5)
O1	0	0.7328(9)	0.25	2.06(2)	0.79(7)
O2	0.042	0.7010(6)	0.5106(3)	54.63(7)	5.11(3)
O3	0.5282(5)	0.1084(8)	0.0721(5)	31.06(7)	4.37(8)
O4	0.2538(4)	0.0548(6)	0.3316(1)	-8.34(8)	0.62(8)
O5	0.3083(9)	0.4033(0)	0.3352(1)	13.83(8)	1.70(1)
O6	0.2028(3)	0.5314(7)	0.4844(1)	-5.15(6)	0.86(9)
O7	0.2914(1)	0.0369(8)	-0.0122(3)	-9.23(3)	0.67(0)
O8	0.3003(7)	0.2378(1)	0.6213(6)	22.73(2)	2.97(5)

Table S3 Bond distance (Å) of $Ba_3LuGa_2O_{7.5}$:0.02Bi^{3+}

Ba1-O1	2.96267(5)	Ba2-O6	2.93374(3)
Ba1-O2	1.94779(3)	Ba2-O7	2.39480(2)
Ba1-O2	3.04842(4)	Ba2-O7	2.90283(3)
Ba1-O6	2.62071(3)	Ba2-O8	1.18302(3)
Ba1-O6	2.91503(3)	（average）	2.636189(2)
Ba1-O7	3.16622(4)	Lu1-O1	2.73256(4)
Ba1-O8	2.18728(4)	Lu1-O2	1.98270(3)
（average）	2.69259(2)	Lu1-O3	1.92192(2)
Ba2-O3	2.92168(4)	Lu1-O4	1.75386(2)
Ba2-O3	2.10881(4)	Lu1-O5	2.13039(2)
Ba2-O4	3.04052(3)	Lu1-O6	2.23874(3)
Ba2-O5	2.97411(3)	（average）	2.12669(7)

Note S1:

The average lifetime $\tau*$ can be calculated by the following formula:

$$\tau^* = \frac{A_1\tau_1^2 + A_2\tau_2^2 + A_3\tau_3^2}{A_1\tau_1 + A_2\tau_2 + A_3\tau_3}$$

(1)

where A_1, A_2 and A_3 are the fitting constants, t is the time, τ_1, τ_2, and τ_3 are the decay time for different components.[1]

Note S2:

A series of BLGO:xBi^{3+} samples were synthesized to determine the optimal doping concentration of Bi^{3+} ions. Fig. S3 exhibits the PL spectra of BLGO:xBi^{3+} ($0.005 \leq x \leq 0.06$) as a function of Bi^{3+} concentration (x) under 351 nm excitation. With Bi^{3+} concentration (x) increasing, PL intensity of BLGO:Bi^{3+} firstly advances and reaches a maximum when Bi^{3+} concentration is 0.02. Then the PL intensity declines gradually with x further rising, which is owing to the concentration quenching effect. The integrated PL intensity varied with Bi^{3+} concentration (x) is shown in the inset of Fig. S4. To investigate the mechanism of concentration quenching for Bi^{3+}-doped BLGO, the critical distance R_c can be estimated by the following equation:[2]

$$R_c \approx 2\left(\frac{3V}{4\pi x_c z}\right)^{1/3} \tag{2}$$

where V represents the cell volume, Z is the number of formula units per unit cell and xc refers to the optimal concentration. For BLGO, V = 863.956 Å3, Z = 4 and x_c is 0.02, so the critical distance R_c of Bi^{3+} ions is calculated to be approximately 27.42 Å, which is longer than the exchange interaction distance (~ 5 Å). Thus, it is unlikely that the concentration quenching between Bi^{3+} ions occurs exchange interaction, and we speculate that multipolar interactions play a major role in the concentration quenching between Bi^{3+} ions. According to Dexter's theory, the multipole interaction mechanism of energy transfer can be determined by using the following expression:[3, 4]

$$I/x = k\left[1 + \beta(x)^{\theta/3}\right]^{-1} \tag{3}$$

where I is the integrated emission intensity, x is the activator ions concentration, k and β are constants in a given host, θ is an indication of electric multipolar character. The noteworthy value is θ, where θ = 6, 8 and 10 correspond to dipole-dipole, dipole-quadrupole, and quadrupole-quadrupole interactions, respectively. As depicted in the inset of Fig. S4, the dependence of Ln (I/x) and Ln (x) can be well-fitted as a line with the slope -2.16, and the θ can be calculated to be approximately 6.48, which is close to 6. Therefore, the result indicates that the concentration quenching between the Bi^{3+} ions occurs via the dipole-dipole interaction.

Note S3:

The absorption efficiency (ξ_{abs}), internal quantum efficiency (IQE) and external quantum efficiency (EQE) can be respectively calculated by the following formula:

$$\xi_{abs} = \frac{\int E_R - \int E_S}{\int E_R} \tag{4}$$

$$IQE = \frac{\int L_S}{\int E_R - \int E_S} \tag{5}$$

$$EQE = IQE \times \xi_{abs} \tag{6}$$

Where $\int L_S$ represents the integral area of emission spectrum, $\int E_R$ and $\int E_S$ represent the integral area of excitation spectrum without and with the phosphor in the integrating sphere, respectively.

[1] S. Wang, H. Wu, Y. Fan, Q. Wang, T. Tan, R. Pang, S. Zhang, D. Li, L. Jiang, C. Li, H. Zhang, *Chem. Eng. J.*, 2022, **432**, 134265.

[2]. G. Blasse, *Phys. Lett. A*, 1969, **24**, 131-&.

[3]. V. Uitert, *J. Electrochem. Soc.*, 1967, **114**, 1048.

[4]. W. Lv, Y. Jia, Q. Zhao, M. Jiao, B. Shao, W. Lü, and H. You, *Adv. Opt. Mater.*, 2014, **2**, 183-188.