

Supplementary information for

Exclusive confinement of Bi³⁺-activators in the triangular prism enabling efficient and thermally stable green emission in tridymite-type phosphor CaBaGa₄O₈:Bi³⁺

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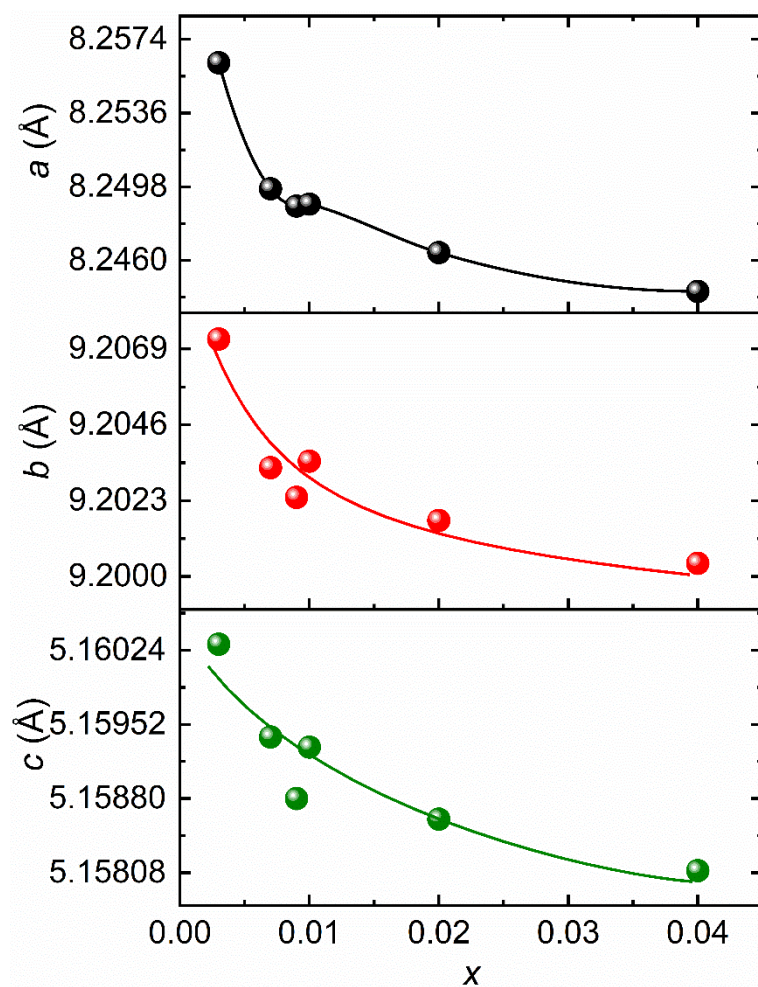


Fig. S1 Plots of lattice parameters of $\text{CaBaGa}_4\text{O}_8:x\text{Bi}^{3+}$ as a function of Bi^{3+} -content (x).

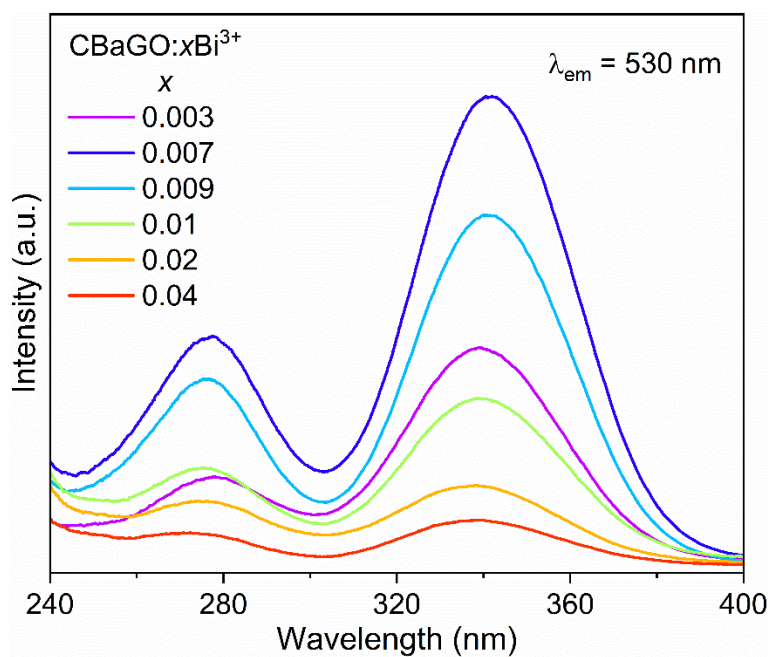


Fig. S2 PLE spectra of $\text{CaBaGa}_4\text{O}_8:x\text{Bi}^{3+}$ recorded with $\lambda_{\text{em}} = 530$ nm.

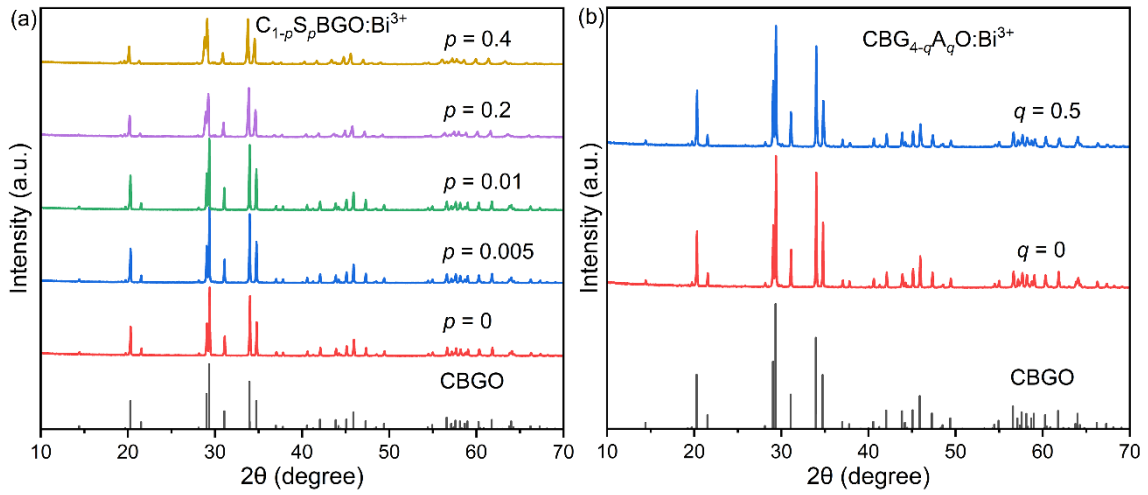


Fig. S3 XRPD patterns for $Ca_{1-p}Sr_pBaGa_4O_8:0.007Bi^{3+}$ ($C_{1-p}S_pBGO:Bi^{3+}$) (a) and $CaBaGa_{4-q}Al_qO_8:0.007Bi^{3+}$ ($CBG_{4-q}A_qO:Bi^{3+}$) (b).

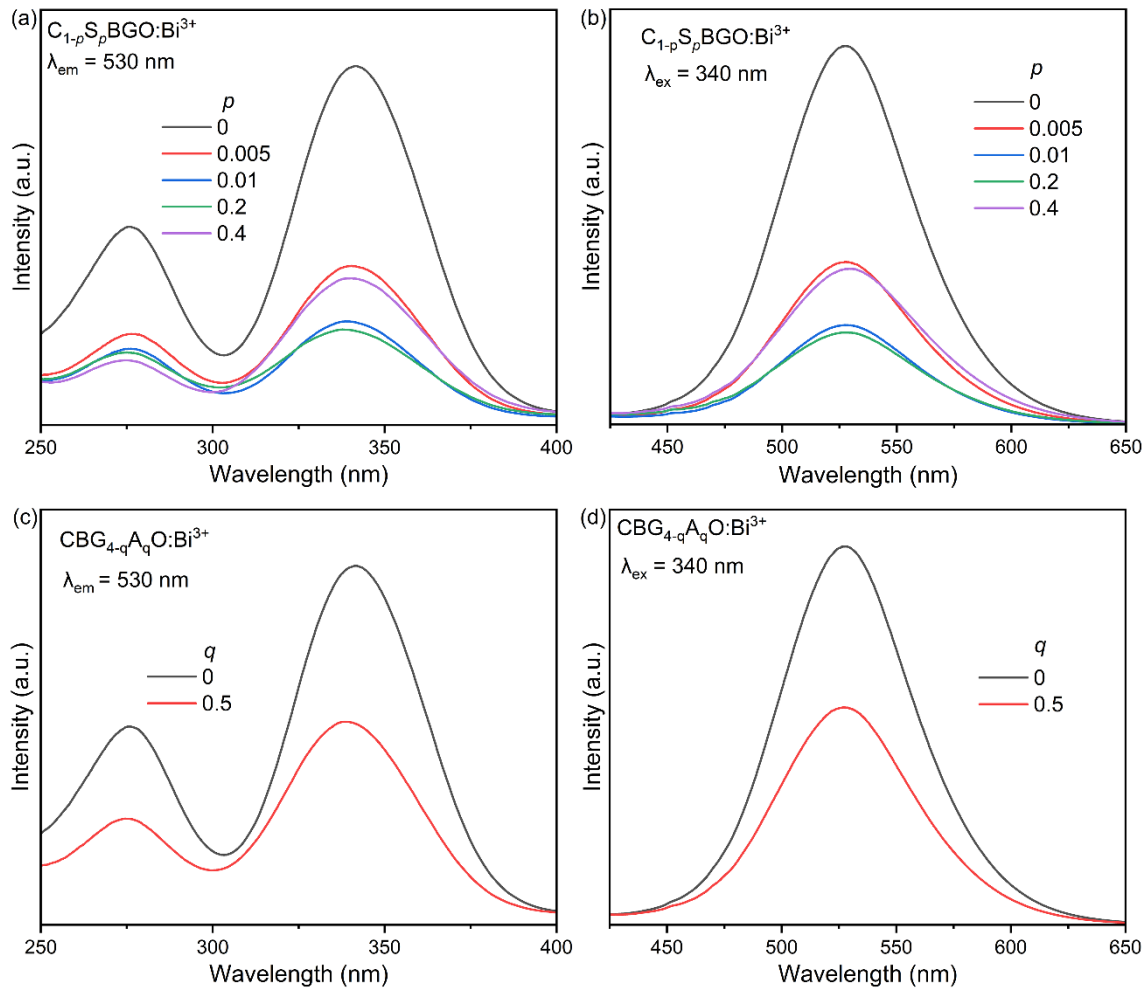


Fig. S4 PLE and PL spectra for $C_{1-p}S_pBGO:Bi^{3+}$ (a, b) and $CBG_{4-q}A_qO:Bi^{3+}$ (c, d).

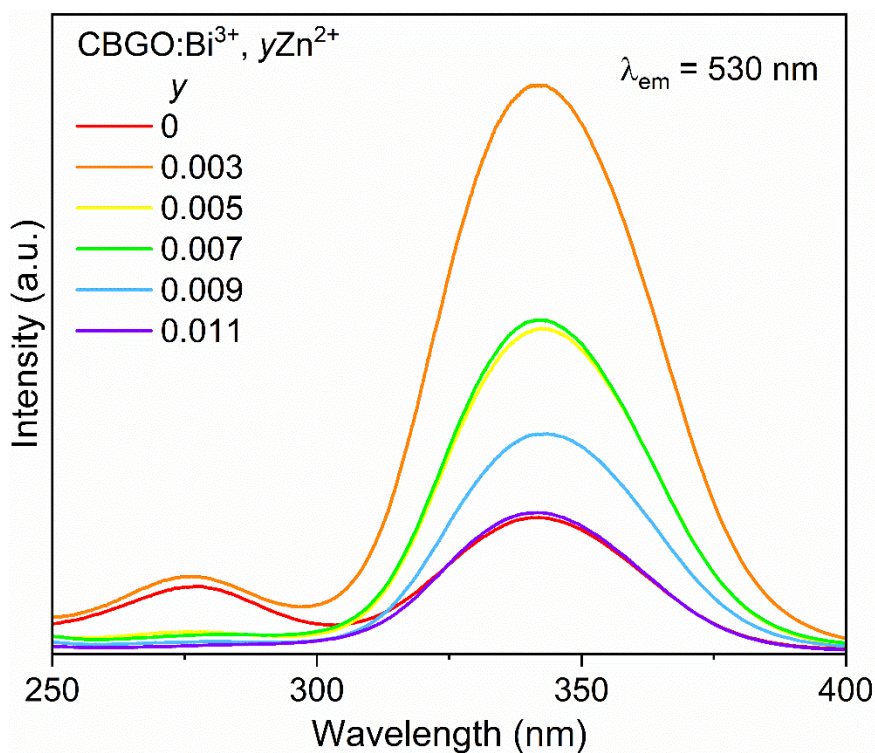


Fig. S5 PLE spectra of $\text{CBGO:Bi}^{3+}, y\text{Zn}^{2+}$ recorded with $\lambda_{\text{em}} = 530 \text{ nm}$.

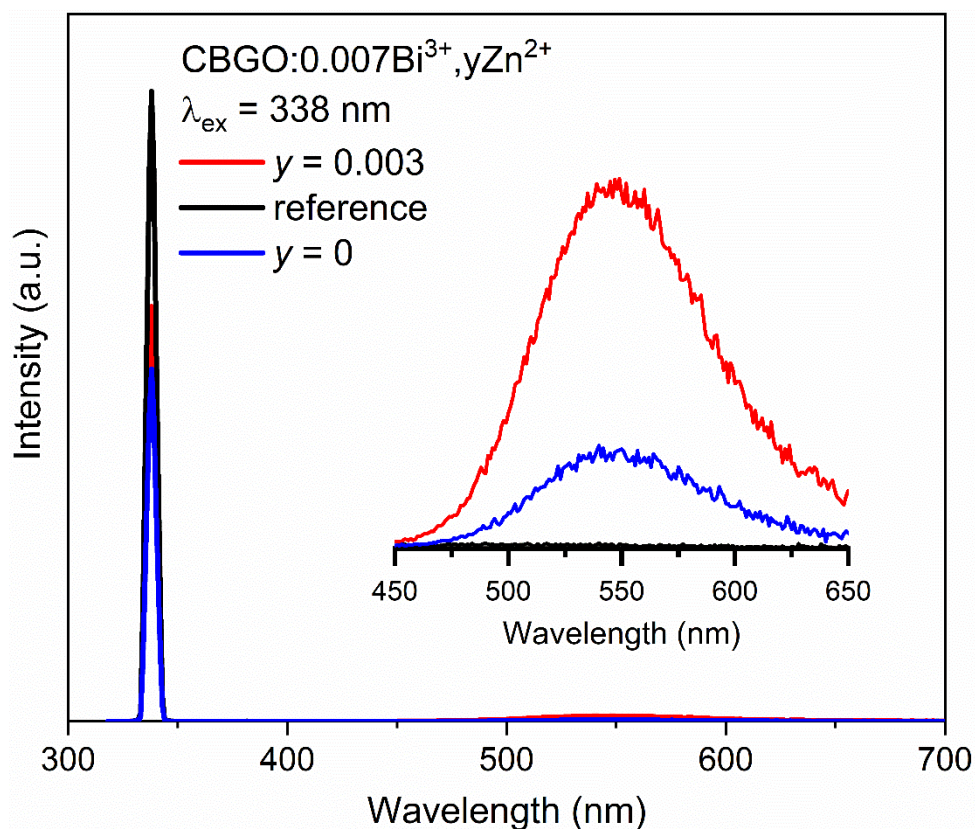


Fig. S6 The optical spectra of $\text{CBGO:0.007Bi}^{3+}, y\text{Zn}^{2+}$ with $y = 0$ and 0.003 phosphors recorded by the quantum efficiency system under the excitation wavelength of 340 nm . The black lines in the figures represents the reflectance of the BaSO_4 standard.

Table S1 Atomic coordinates, site occupancy factor (*sof.*), isotropic thermal displacement factors for CaBaGa₄O₈:0.01Bi³⁺ and CaBaGa₄O₈:0.007Bi³⁺, 0.003Zn²⁺ obtained from Rietveld refinements against high-resolution Cu K_{α1} XRPD data.

CaBaGa ₄ O ₈ :0.01Bi ³⁺						
Atom	site	<i>x</i>	<i>y</i>	<i>z</i>	<i>sof.</i>	Beq. (Å ²)
Ca	2a	0	0.5	0.4258(5)	0.99	1.3(1)
Bi	2a	0	0.5	0.4258(5)	0.01	1.3(1)
Ba	2a	0	0	0	1	0.98(3)
Ga	8e	0.29176(9)	0.16730(9)	0.4516(3)	1	0.64(2)
O1	8e	0.2957(6)	0.1655(6)	0.0924(9)	1	0.7(1)
O2	4d	0	0.3288(7)	0.077(1)	1	0.4(1)
O3	4c	0.1891(9)	0	0.566(1)	1	1.0(2)
CaBaGa ₄ O ₈ :0.007Bi ³⁺ ,0.003Zn ²⁺						
Atom	site	<i>x</i>	<i>y</i>	<i>z</i>	<i>sof.</i>	Beq. (Å ²)
Ca	2a	0	0.5	0.4261(6)	0.993	1.2(1)
Bi	2a	0	0.5	0.4261(6)	0.007	1.2(1)
Ba	2a	0	0	0	1	0.97(3)
Ga/Zn	8e	0.2919(1)	0.1671(1)	0.4519(3)	0.997/0.003	0.68(3)
O1	8e	0.2954(7)	0.1674(7)	0.092(1)	1	0.5(1)
O2	4d	0	0.3289(9)	0.078(2)	1	0.3(1)
O3	4c	0.191(1)	0	0.564(2)	1	0.7(2)

Table S2 Selected interatomic distances in $\text{CaBaGa}_4\text{O}_8:0.01\text{Bi}^{3+}$ and $\text{CaBaGa}_4\text{O}_8:0.007\text{Bi}^{3+},0.003\text{Zn}^{2+}$ obtained from Rietveld refinements against high-resolution $\text{Cu K}\alpha_1$ XRPD data.

$\text{CaBaGa}_4\text{O}_8:0.01\text{Bi}^{3+}$					
bond	length (Å)	bond	length (Å)	bond	length (Å)
Ga–O2	1.837(3)	Ca–O2 × 2	2.393(7)	Ba–O3 × 2	2.732(7)
Ga–O1	1.849(5)	Ca–O1 × 4	2.430(5)	Ba–O1 × 4	2.917(5)
Ga–O1	1.854(5)			Ba–O2 × 4	3.053(6)
Ga–O3	1.854(4)			Ba–O3 × 4	3.309(7)
$\text{CaBaGa}_4\text{O}_8:0.007\text{Bi}^{3+},0.003\text{Zn}^{2+}$					
bond	length (Å)	bond	length (Å)	bond	length (Å)
Ga–O2	1.835(6)	Ca–O2 × 2	2.389(8)	Ba–O3 × 2	2.749(9)
Ga–O1	1.837(3)	Ca–O1 × 4	2.442(6)	Ba–O1 × 4	2.923(6)
Ga–O1	1.857(6)			Ba–O2 × 4	3.055(8)
Ga–O3	1.842(5)			Ba–O3 × 2	3.309(9)