Computational descriptions

The crystallographic data of compound $Na_3GdB_8O_{15}$ from SC-XRD analysis were used for computational study without geometry optimization. The calculation (CASTEP code) employs pseudo-potentials to describe electron-ion interactions and uses a plane-wave basis set for electronic wave functions [1]. The Generalized Gradient Approximation (GGA) with the Perdew−Burke−Ernzerhof (PBE) functional was used for the potential exchange-correlation [2]. A plane-wave basis set energy cutoff was 820 eV within the norm-conserving pseudo-potential [3]. The total energy and the force convergence thresholds were 1.0×10^{-6} eV/atom and 0.05 eV/Å, respectively. The *k*-point set meshes to define the number of integration points that will be used to integrate the wave function in reciprocal space were $4 \times 4 \times 2$ for calculating band structure and density of state. The rest parameters used in the calculations were set by the default values of the CASTEP code. Pseudo atomic calculations were performed for, Na-$2s^2 2s^6 3p^1$, Gd-$4f^7 5s^2 5p^6 5d^1$, B-$2s^2 2p^1$ and O-$2s^2 2p^4$, respectively.

[1] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson, M. C. Payne, First principles methods using CASTEP, Z. Krist-Cryst. Mater. 220 (2005) 567-570.

[2] Y. Zhang, J. Sun, J. P. Perdew, X. Wu, Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA, Phys. Rev. B 96 (2017) 035143-035158.

[3] V. Milman, K. Refson, S. J. Clark, C. J. Pickard, J. R. Yates, S. P. Gao, P. J. Hasnip, M. I. J. Probert, A. Perlov, M.D. Segall, Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation, J. Mol. Struc: Theochem. 954 (2010) 22-35.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of $Na_3GdB_8O_{15}$.

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.6340 (3)	0.3864 (2)	0.22853 (12)	0.0231 (3)
Na2	0.0920 (3)	0.3120 (2)	0.10828 (10)	0.0209 (3)
Na3	0.7487 (2)	0.2624 (2)	0.52279 (11)	0.0211 (3)
Gd1	0.91893 (2)	0.24898 (2)	0.83231 (2)	0.00530 (6)
B1	0.3803 (6)	0.6358 (5)	−0.0011 (3)	0.0083 (6)
B2	0.7276 (6)	0.9418 (5)	0.0134 (3)	0.0084 (6)
B3	0.6116 (6)	0.7971 (5)	0.1727 (2)	0.0065 (6)
B4	0.6280 (6)	1.0168 (5)	0.3139 (3)	0.0081 (6)
B5	0.8947 (6)	0.8478 (5)	0.3410 (2)	0.0065 (6)
B6	0.7960 (6)	0.7174 (5)	0.5117 (3)	0.0079 (6)
B7	0.6848 (6)	0.8702 (5)	0.6430 (2)	0.0062 (6)
B8	0.8341 (6)	0.6091 (5)	0.6802 (3)	0.0084 (6)
O1	0.8377 (4)	0.5874 (3)	0.57699 (16)	0.0101 (4)

O2	0.5574 (4)	1.1485 (3)	0.35225 (16)	0.0085 (4)
O3	0.8304 (4)	1.0075 (3)	0.36197 (15)	0.0079 (4)
O4	0.7826 (4)	0.9290 (3)	0.11684 (16)	0.0098 (4)
O5	0.5488 (4)	0.7775 (3)	−0.04565 (16)	0.0127 (5)
O6	0.8745 (4)	0.7215 (3)	0.42408 (15)	0.0087 (4)
O7	0.7443 (4)	0.7204 (3)	0.24680 (15)	0.0065 (4)
O8	0.1968 (4)	0.4940 (3)	−0.05969 (17)	0.0133 (5)
O9	1.1442 (4)	0.9260 (3)	0.32523 (16)	0.0074 (4)
O10	0.7384 (4)	0.7327 (3)	0.71033 (15)	0.0084 (4)
O11	0.6743 (4)	0.8204 (3)	0.53601 (15)	0.0077 (4)
O12	0.4083 (4)	0.6447 (3)	0.10459 (15)	0.0083 (4)
O13	0.9241 (4)	0.5126 (3)	0.74583 (16)	0.0109 (4)
O14	0.5011 (4)	0.9045 (3)	0.22464 (16)	0.0090 (4)
O15	0.8404 (4)	1.1017 (3)	−0.02783 (16)	0.0117 (4)

Table S2. Atomic displacement parameters (Å^2) of $Na_3GdB_8O_{15}$.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0195 (7)	0.0154 (7)	0.0373 (9)	0.0063 (6)	0.0141 (6)	0.0102 (6)
Na2	0.0267 (8)	0.0196 (7)	0.0132 (7)	0.0076 (6)	0.0008 (6)	−0.0047 (5)
Na3	0.0158 (7)	0.0250 (8)	0.0220 (8)	0.0118 (6)	−0.0050 (6)	−0.0067 (6)
Gd1	0.00525 (8)	0.00582 (8)	0.00440 (8)	0.00185 (5)	0.00091 (5)	0.00051 (5)
B1	0.0097 (16)	0.0098 (16)	0.0071 (15)	0.0060 (13)	0.0010 (12)	0.0019 (12)
B2	0.0076 (15)	0.0114 (16)	0.0078 (16)	0.0053 (13)	0.0024 (12)	0.0009 (12)
B3	0.0062 (15)	0.0063 (15)	0.0057 (15)	0.0014 (12)	0.0008 (12)	−0.0019 (12)
B4	0.0092 (16)	0.0071 (15)	0.0081 (15)	0.0021 (13)	0.0045 (12)	0.0028 (12)
B5	0.0079 (15)	0.0074 (15)	0.0050 (15)	0.0043 (12)	0.0006 (12)	0.0000 (12)
B6	0.0079 (16)	0.0077 (15)	0.0078 (15)	0.0034 (13)	0.0002 (12)	0.0010 (12)
B7	0.0062 (15)	0.0070 (15)	0.0060 (15)	0.0032 (12)	0.0009 (12)	0.0003 (11)
B8	0.0092 (16)	0.0072 (15)	0.0091 (16)	0.0027 (13)	0.0035 (13)	0.0025 (12)
O1	0.0162 (11)	0.0109 (10)	0.0067 (10)	0.0086 (9)	0.0034 (8)	0.0015 (8)
O2	0.0050 (10)	0.0100 (10)	0.0117 (11)	0.0040 (8)	0.0025 (8)	−0.0001 (8)
O3	0.0066 (10)	0.0100 (10)	0.0076 (10)	0.0049 (8)	−0.0005 (8)	−0.0016 (8)
O4	0.0084 (10)	0.0117 (10)	0.0069 (10)	0.0014 (8)	0.0021 (8)	0.0016 (8)
O5	0.0131 (11)	0.0119 (11)	0.0082 (11)	0.0003 (9)	0.0017 (9)	0.0001 (8)
O6	0.0127 (11)	0.0107 (10)	0.0053 (10)	0.0071 (9)	0.0025 (8)	0.0023 (8)
O7	0.0072 (10)	0.0074 (10)	0.0050 (10)	0.0040 (8)	−0.0005 (8)	−0.0004 (8)
O8	0.0113 (11)	0.0121 (11)	0.0109 (11)	−0.0001 (9)	0.0004 (9)	−0.0030 (8)
O9	0.0050 (10)	0.0068 (10)	0.0110 (10)	0.0028 (8)	0.0022 (8)	−0.0008 (8)
O10	0.0115 (11)	0.0104 (10)	0.0066 (10)	0.0074 (9)	0.0027 (8)	0.0016 (8)
O11	0.0085 (10)	0.0115 (10)	0.0054 (10)	0.0065 (8)	0.0011 (8)	0.0005 (8)
O12	0.0064 (10)	0.0083 (10)	0.0076 (10)	0.0006 (8)	0.0005 (8)	0.0001 (8)
O13	0.0156 (11)	0.0132 (11)	0.0085 (10)	0.0095 (9)	0.0048 (9)	0.0048 (8)
O14	0.0067 (10)	0.0124 (11)	0.0084 (10)	0.0054 (9)	−0.0006 (8)	−0.0032 (8)
O15	0.0110 (11)	0.0121 (11)	0.0111 (11)	0.0031 (9)	0.0036 (9)	0.0049 (9)

Table S3. Two phase riveted refinement of $Na_3GdB_8O_{15}$ and $GdBO_3$.

Two-phase refinement	$Na_3GdB_8O_{15}$	$GdBO_3$
Crystal system, space group	Triclinic, *P*-1	Hexagonal, $P6_3/mmc$
Unit cell (Å, °)	a = 6.27955(16)	a = 3.83211(24)
	b = 7.53038(18)	c = 8.9002(9)
	c = 13.47030(30)	
	α = 90.5311(18)	
	β = 100.6295(19)	
	γ = 113.5014(14)	
Cell volume (Å^3)	571.686(23)	113.189(17)
2θ-interval, °	10−75°	
Wt %	0.97512	0.024877
R_{wp} (%)	6.00	
R_p (%)	4.90	
χ^2	1.447	

Table S4. IQY and EQY of the $Na_3Gd_{0.98-y}Y_yCe_{0.02}B_8O_{15}$ phosphors.

$Na_3Gd_{0.98-y}Y_yB_8O_{15}$:0.02$Ce^{3+}$	IQY (%)	EQY (%)
y = 0	8.43	3.49
y = 0.1	11.26	4.76
y = 0.2	11.99	4.99
y = 0.3	12.58	5.09
y = 0.4	12.98	5.65
y = 0.5	10.61	5.20

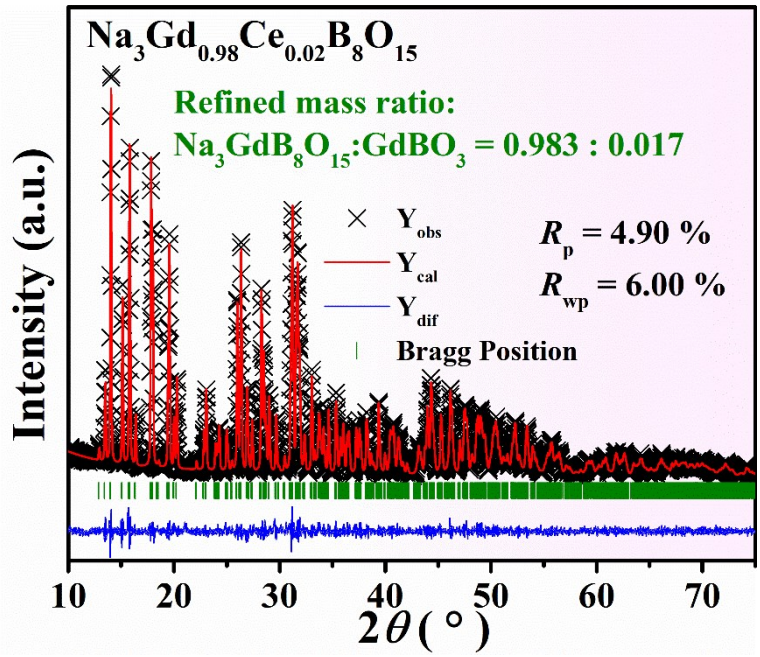

Figure S1. Rietveld refinement of $Na_3Gd_{0.98}Ce_{0.02}B_8O_{15}$ powder

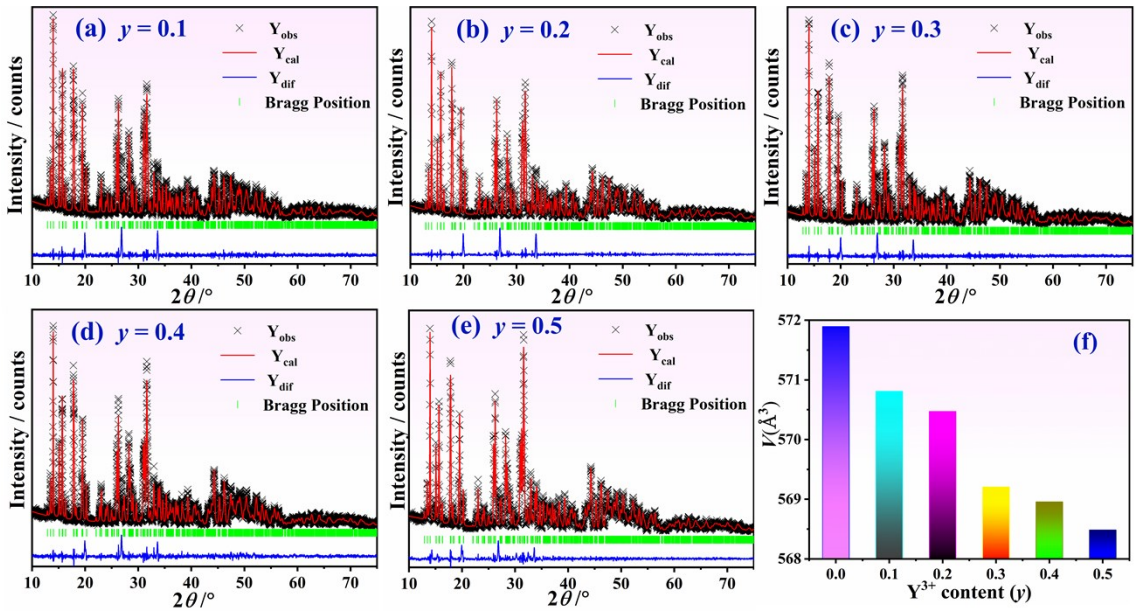

Figure S2. Rietveld refinement of powder XRD pat-terns of $Na_3Gd_{0.98-y}Y_yCe_{0.02}B_8O_{15}$: (a) y = 0.1, (b) y = 0.2, (c) y = 0.3, (d) y = 0.4, (e) y = 0.5. (f) Cell parameters versus Y content y

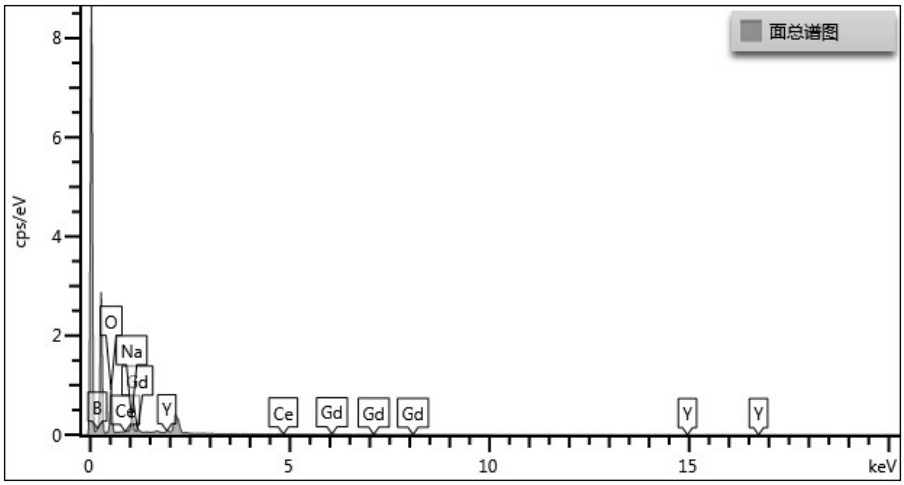

Figure S3. EDS analysis of $Na_3Gd_{0.58}Y_{0.4}Ce_{0.02}B_8O_{15}$

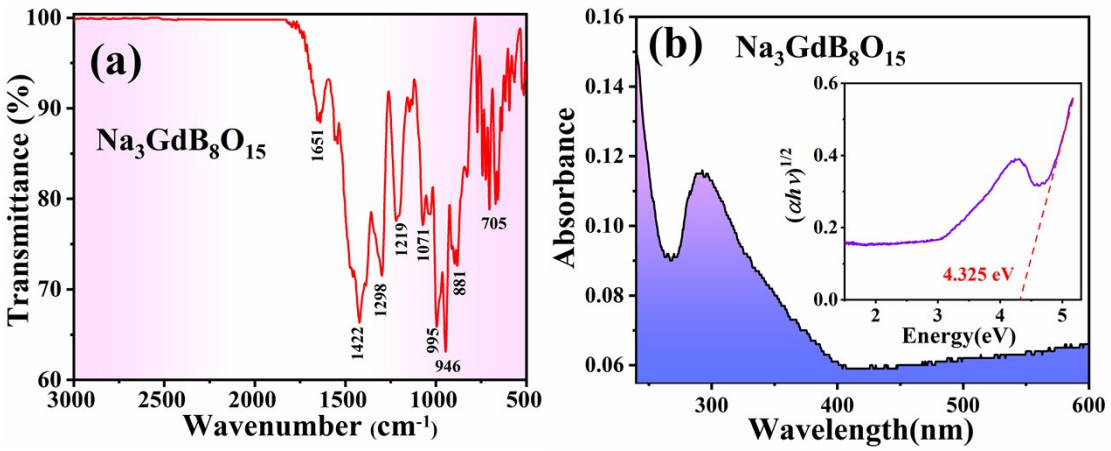

Figure S4. (a) IR spectrum of $Na_3GdB_8O_{15}$. (b) UV–Vis absorption spectrum of $Na_3GdB_8O_{15}$

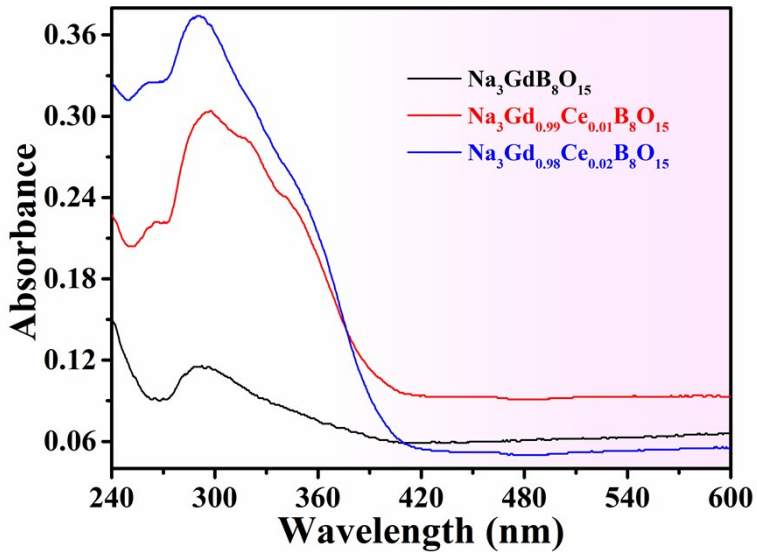

Figure S5. UV–Vis absorption spectrum of $Na_3Gd_{1-x}Ce_xB_8O_{15}$ (x = 0, 0.01, 0.02)

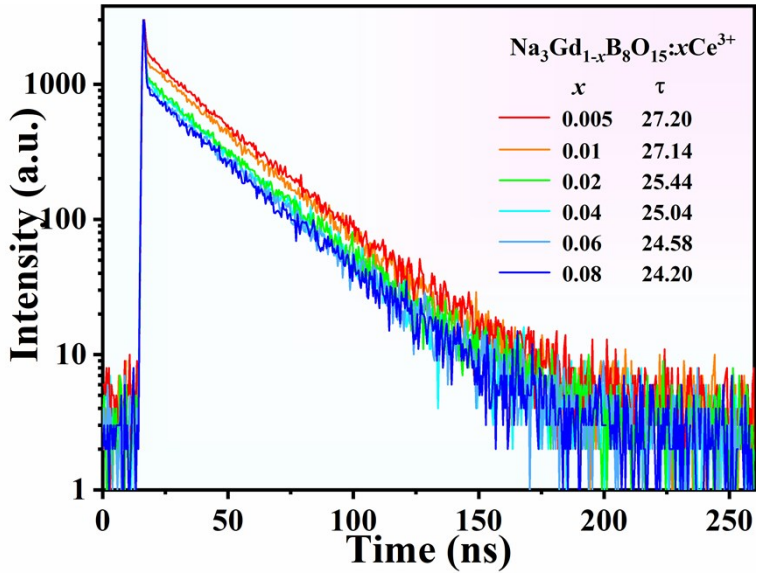

Figure S6. Decay curves (λ_{ex} = 365 nm, λ_{em} = 412 nm) and fitting lifetimes of $Na_3Gd_{1-x}Ce_xB_8O_{15}$ (x = 0.005 ~ 0.08) phosphors

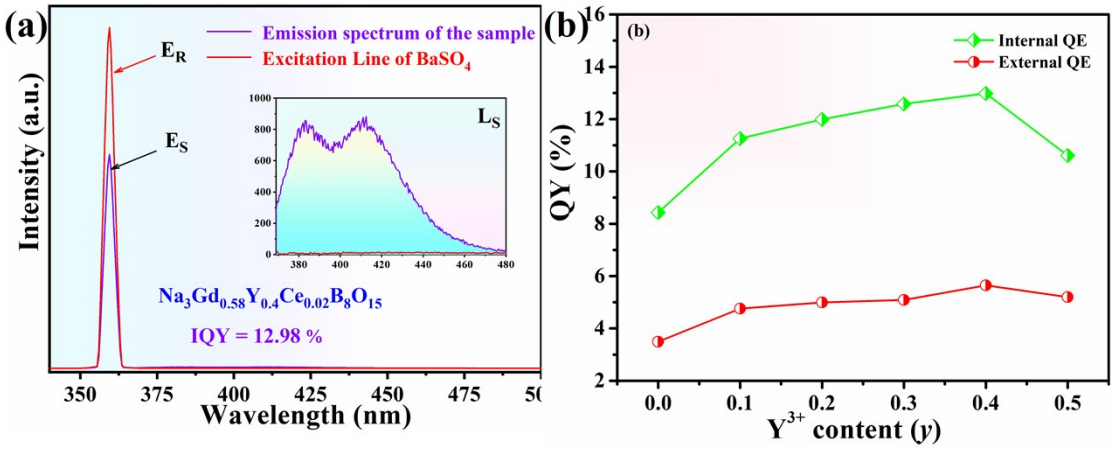

Figure S7. (a) Excitation profile of $BaSO_4$ and the PL spectra of the $Na_3Gd_{0.58}Y_{0.4}Ce_{0.02}B_8O_{15}$ phosphor collected by using an integrating sphere. (b) The internal and external quantum yields (QE) of $Na_3Gd_{0.98-y}Y_yCe_{0.02}B_8O_{15}$ (y = 0, 0.1, 0.2, 0.3, 0.4, 0.5)