Supporting information

Layered structure-induced quenching delay toward highly efficient and thermally stable red emission in Eu^{3+}-activated borotellurate phosphor

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Table S1 Rietveld refinement results of the NYTB:xEu^{3+} samples.

Sample	Space group	Cell parameters (Å), Cell Volume (Å^3)	R_{wp}, R_p, χ^2
$x = 0$	P2$_1$/c	$a = 6.309730$ $b = 9.934610$ $c = 6.730189$ $V = 408.944$	6.19%, 4.68%, 0.65
$x = 0.1$	P2$_1$/c	$a = 6.313962$ $b = 9.946430$ $c = 6.736743$ $V = 410.052$	8.39%, 6.39%,0.96
$x = 0.2$	P2$_1$/c	$a = 6.316231$ $b = 9.952826$ $c = 6.741315$ $V = 410.695$	9.25%, 6.99%, 1.14
$x = 0.3$	P2$_1$/c	$a = 6.317928$ $b = 9.961890$ $c = 6.746250$ $V = 411.434$	9.30%, 6.86%, 1.10
$x = 0.4$	P2$_1$/c	$a = 6.318399$ $b = 9.973191$ $c = 6.751103$ $V = 412.137$	9.32%, 6.82%, 1.07
$x = 0.5$	P2$_1$/c	$a = 6.320568$ $b = 9.978502$ $c = 6.753164$ $V = 412.576$	9.75%, 7.03%, 0.99
$x = 0.6$	P2$_1$/c	$a = 6.322726$ $b = 9.985598$ $c = 6.757085$ $V = 413.266$	9.92%, 7.41%, 1.05
$x = 0.7$	P2$_1$/c	$a = 6.324495$ $b = 9.989513$ $c = 6.671006$ $V = 413.723$	9.35%, 6.76%, 1.07

Table S2 Atomic coordinates, occupation factors and displacement parameters of NYTB:xEu^{3+} samples.

Atom	Wyck.	x/a	y/b	z/c	Occ.	U_{iso} (Å^2)
			$x = 0$			
Na	4e	-0.4159	0.6108	0.166	1	0.01007
Y	4e	0.1267	0.8337	0.0239	1	0.00993
Te	2c	0.0000	0.5000	0.0000	1	0.01085
B	4e	0.3364	0.3996	0.3711	1	0.0086
O1	4e	0.481	0.8267	0.0561	1	0.02485
O2	4e	-0.0049	0.6494	0.176	1	0.0097
O3	4e	0.2891	0.4386	0.1636	1	0.02152
O4	4e	-0.1998	0.9377	0.0083	1	0.02457
O5	4e	-0.1622	0.3855	0.1338	1	0.00804
			$x = 0.1$			
Na	4e	-0.4159	0.6108	0.166	1	0.01144
Y	4e	0.1295	0.8339	0.02389	0.95	0.00937
Eu	4e	0.1295	0.8339	0.02389	0.05	0.00937
Te	2c	0	0.5	0	1	0.00397
B	4e	0.3364	0.3996	0.3711	1	0.02433
O1	4e	0.481	0.8267	0.0561	1	0.02615
O2	4e	-0.0049	0.6494	0.176	1	0.01264
O3	4e	0.2891	0.4386	0.1636	1	0.01115
O4	4e	-0.1998	0.9377	0.0083	1	0.02262
O5	4e	-0.1622	0.3855	0.1338	1	0.01388
			$x = 0.2$			
Na	Na	-0.4159	0.6108	0.166	1	0.02756
Y	Y	0.12932	0.83357	0.02356	0.9	0.00753
Eu	Eu	0.12932	0.83357	0.02356	0.1	0.00753
Te	Te	0	0.5	0	1	0.03944
B	B	0.3364	0.3996	0.3711	1	0.0292
O1	O1	0.481	0.8267	0.0561	1	0.03414
O2	O2	-0.0049	0.6494	0.176	1	0.08953
O3	O3	0.2891	0.4386	0.1636	1	0.10385
O4	O4	-0.1998	0.9377	0.0083	1	0.09276
O5	4e	-0.1622	0.3855	0.1338	1	0.04774
			$x = 0.3$			
Na	Na	-0.4159	0.6108	0.166	1	0.00918
Y	Y	0.12706	0.83391	0.02114	0.85	0.00475
Eu	Eu	0.12706	0.83391	0.02114	0.15	0.00475
Te	Te	0	0.5	0	1	0.00178
B	B	0.3364	0.3996	0.3711	1	0.0086

O1	O1	0.481	0.8267	0.0561	1	0.0125
O2	O2	-0.0049	0.6494	0.176	1	0.0097
O3	O3	0.2891	0.4386	0.1636	1	0.0125
O4	O4	-0.1998	0.9377	0.0083	1	0.0104
O5	4e	-0.1622	0.3855	0.1338	1	0.0098
x = 0.4						
Na	Na	-0.4159	0.6108	0.166	1	0.0104
Y	Y	0.12763	0.83378	0.02269	0.8	0.00428
Eu	Eu	0.12763	0.83378	0.02269	0.2	0.00428
Te	Te	0	0.5	0	1	0.00599
B	B	0.3364	0.3996	0.3711	1	0.0086
O1	O1	0.481	0.8267	0.0561	1	0.0124
O2	O2	-0.0049	0.6494	0.176	1	0.0115
O3	O3	0.2891	0.4386	0.1636	1	0.0107
O4	O4	-0.1998	0.9377	0.0083	1	0.0137
O5	4e	-0.1622	0.3855	0.1338	1	0.0066
x = 0.5						
Na	4e	-0.4159	0.6108	0.166	1	0.02529
Y	4e	0.12569	0.83283	0.02129	0.75	0.00406
Eu	4e	0.12569	0.83283	0.02129	0.25	0.00406
Te	2c	0	0.5	0	1	0.0048
B	4e	0.3364	0.3996	0.3711	1	0.0086
O1	4e	0.481	0.8267	0.0561	1	0.0125
O2	4e	-0.0049	0.6494	0.176	1	0.0097
O3	4e	0.2891	0.4386	0.1636	1	0.0125
O4	4e	-0.1998	0.9377	0.0083	1	0.0104
O5	4e	-0.1622	0.3855	0.1338	1	0.0098
x = 0.6						
Na	4e	-0.4159	0.6108	0.166	1	0.04069
Y	4e	0.12397	0.83475	0.02104	0.7	0.00356
Eu	4e	0.12397	0.83475	0.02104	0.3	0.00356
Te	2c	0	0.5	0	1	0.01397
B	4e	0.3364	0.3996	0.3711	1	0.12041
O1	4e	0.481	0.8267	0.0561	1	0.01081
O2	4e	-0.0049	0.6494	0.176	1	0.00819
O3	4e	0.2891	0.4386	0.1636	1	0.8
O4	4e	-0.1998	0.9377	0.0083	1	0.07474
O5	4e	-0.1622	0.3855	0.1338	1	0.02324
x = 0.7						
Na	4e	-0.4159	0.6108	0.166	1	0.02256
Y	4e	0.12787	0.83327	0.02374	0.65	0.0034
Eu	4e	0.12787	0.83327	0.02374	0.35	0.0034
Te	2c	0	0.5	0	1	0.0137
B	4e	0.3364	0.3996	0.3711	1	0.02796

O1	4e	0.481	0.8267	0.0561	1	0.021
O2	4e	-0.0049	0.6494	0.176	1	0.02035
O3	4e	0.2891	0.4386	0.1636	1	0.0458
O4	4e	-0.1998	0.9377	0.0083	1	0.02778
O5	4e	-0.1622	0.3855	0.1338	1	0.01805

Table S3 Chromaticity coordinates and color purity (CP) for NYTB:xEu^{3+} ($x = 0.1$– 0.7).

x	Coordinates (x, y)	CP (%)
0.1	(0.6650, 0.3343)	96.7
0.2	(0.6649, 0.3343)	96.7
0.3	(0.6646, 0.3346)	96.6
0.4	(0.6653, 0.3340)	96.8
0.5	(0.6662, 0.3332)	97.0
0.6	(0.6657, 0.3338)	96.9
0.7	(0.6659, 0.3336)	96.9

Table S4 Chromaticity parameters of the fabricated w-LED as a function of driving current.

Current (mA)	Coordinates (x,y)	CCT (K)	R_a
20	(0.3791,0.3810)	4068	83.0
40	(0.3784,0.3794)	4075	82.7
60	(0.3778,0.3791)	4090	82.8
80	(0.3774,0.3783)	4094	82.9
100	(0.3765,0.3770)	4111	82.6
140	(0.3753,0.3754)	4133	82.7
180	(0.3746,0.3739)	4145	82.2
220	(0.3741,0.3723)	4145	820.
260	(0.3738,0.3705)	4142	82.0
300	(0.3734,0.3674)	4132	81.4

Fig. S1 XRD patterns of the NYTB host (a) sintered at 780 °C with different times and (b) sintered at different temperatures for 30 min.
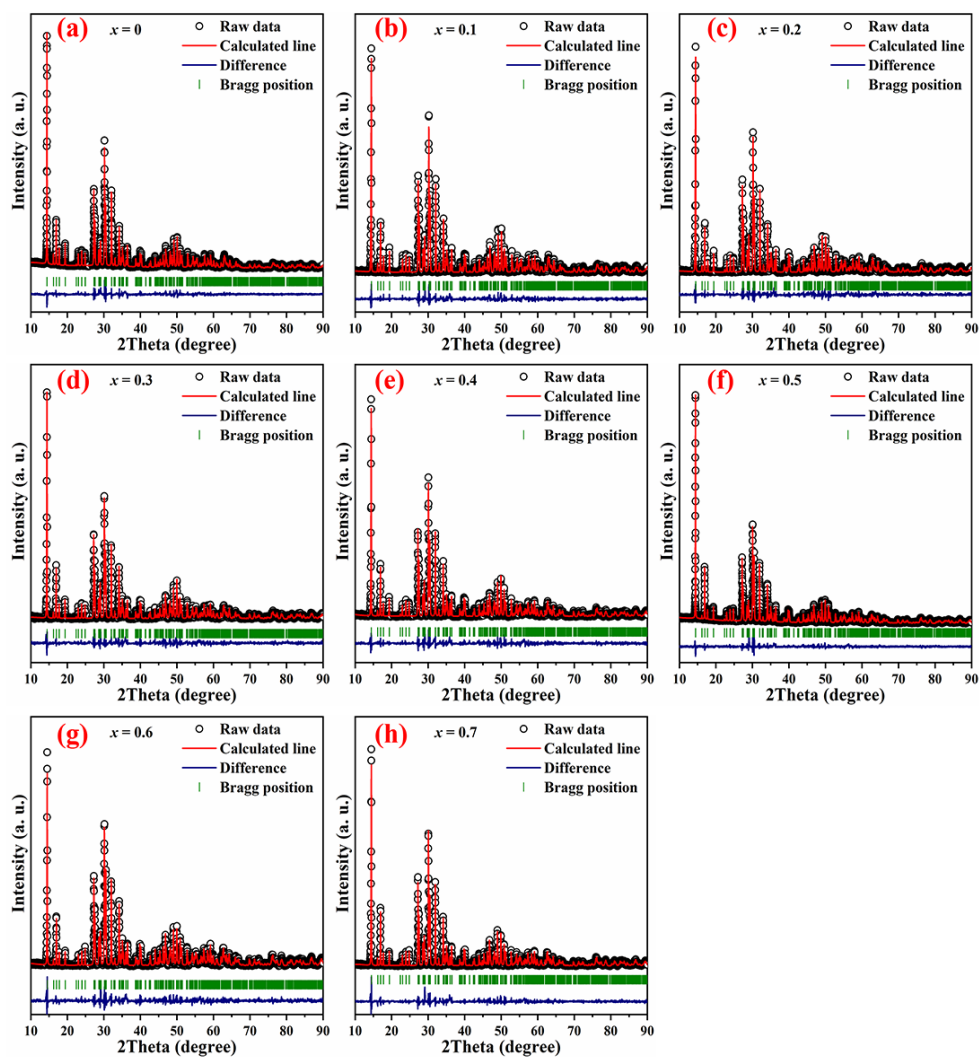

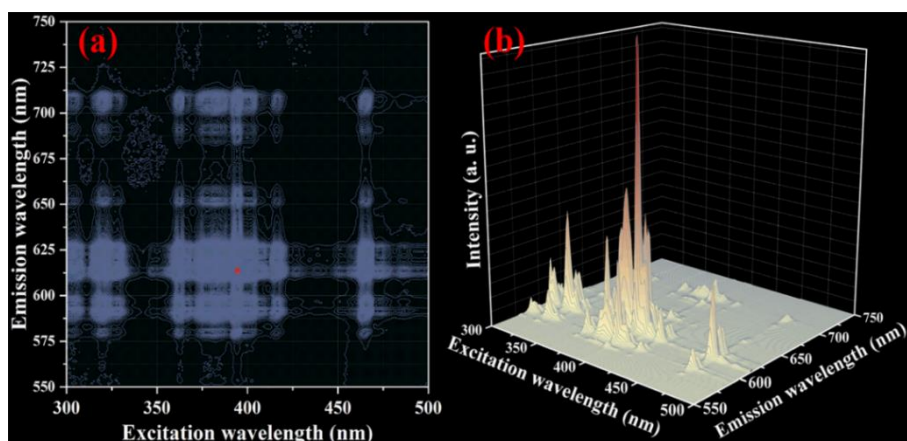**Fig. S2** Rietveld XRD refinements for NYTB:xEu^{3+} (x = 0–0.7).

Fig. S3 (a) Contour line and (b) 3D PL spectra of NYTB:0.5Eu^{3+} under various excitation wavelengths.
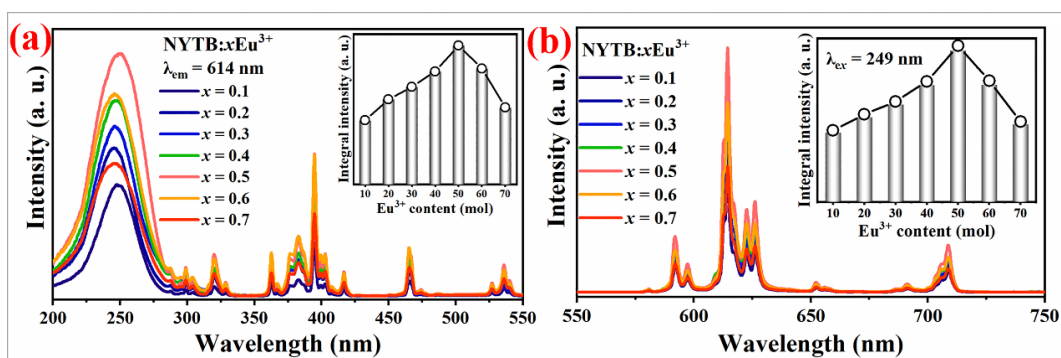

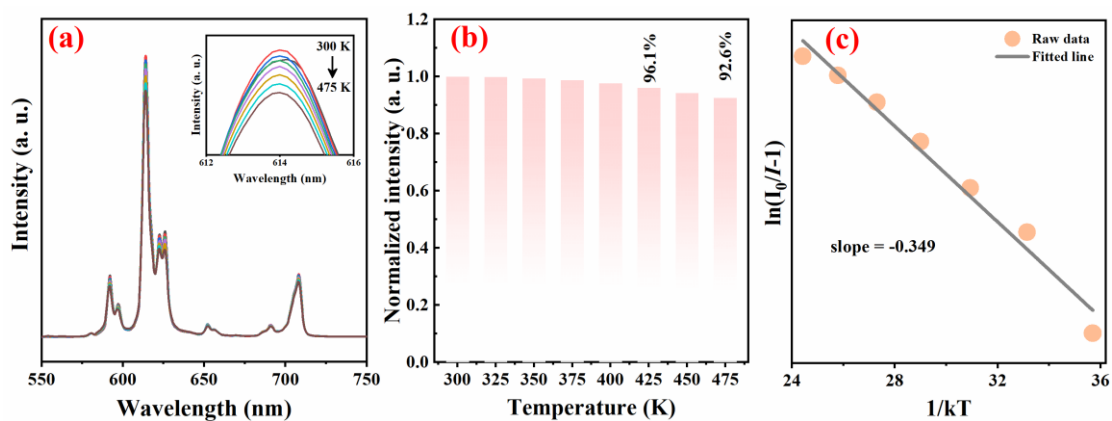**Fig. S4** (a) PLE spectra and (b) PL emission spectra of NYTB:xEu^{3+} (Inset shows integral intensity in response to the Eu^{3+} concentration).

Fig. S5 (a) Temperature-dependent PL of NYTB:0.4Eu^{3+}. (b) Normalized intensity as a function of temperature. (c) Plot of $1/kT$ versus $\ln(I_0/I\text{-}1)$).
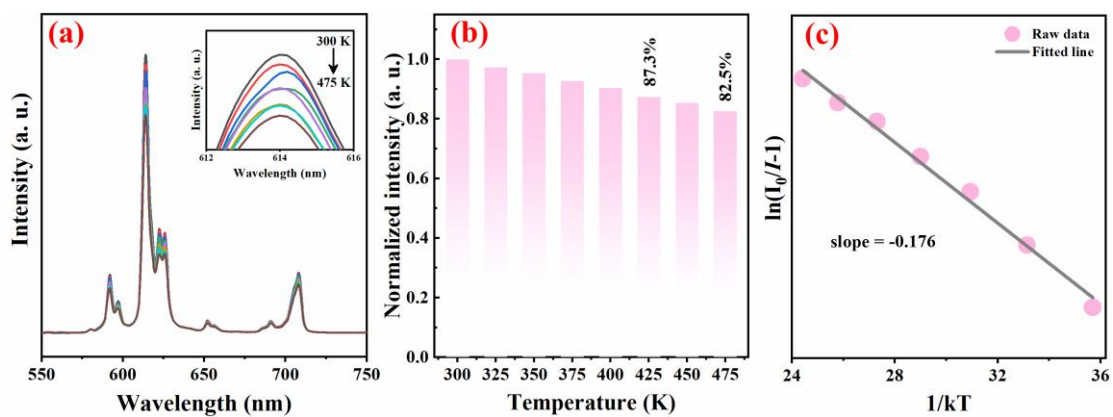
Fig. S6 (a) Temperature-dependent PL of NYTB:0.6Eu^{3+}. (b) Normalized intensity as a function of temperature. (c) Plot of $1/kT$ versus $\ln(I_0/I\text{-}1)$).
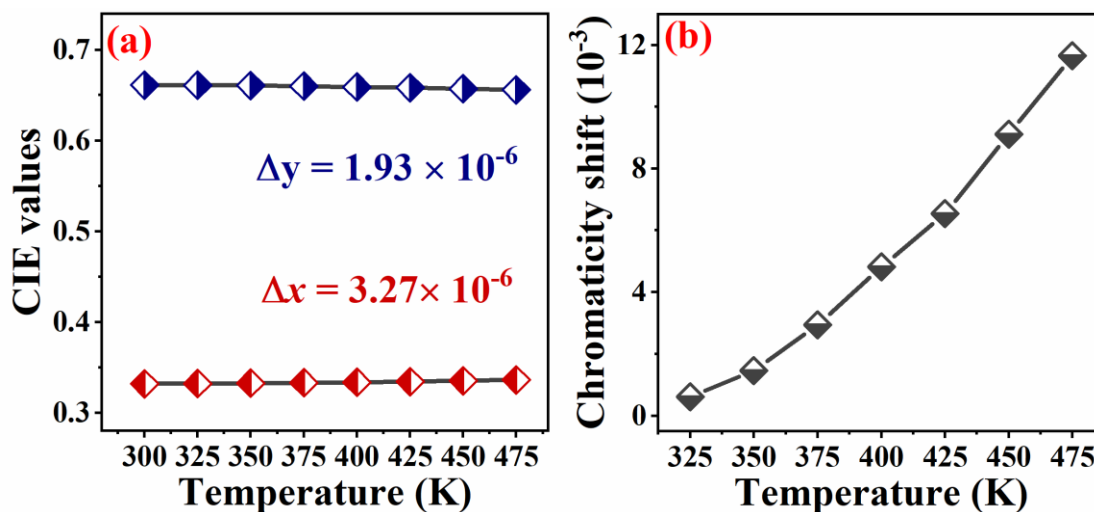

Fig. S7 (a) Temperature-dependent CIE (x, y) values and (b) Temperature-dependent chromaticity shift.

Formula S1:

The E_g values of the NYTB:xEu^{3+} (x = 0 and 0.5) samples are estimated by the Tauc relation:[1]

$$[F(R)h\nu]^{1/n} = A(h\nu - E_g) \tag{S1}$$

where R, A, and hν represent reflectance, absorption, and photon energy, respectively. The n values of 1/2 and 2 correspond to direct and indirect allowed transitions, separately. The NYTB host belongs to an indirect-gap crystal, indicating that the n value is 2.

Formula S2:

Based on Ozawa's theory, the initial quenching concentration is estimated by $1/(1 + z)$, in which z is the number of closest cations around luminescence centers. The emission intensity (I) and doping concentration (x) can be determined by the following formula:[2]

$$\ln\left(\frac{I}{x}\right) = zln(1 - x)C \tag{S2}$$

where C is a constant. The value of z can be achieved by the slope of $\ln(I/x)$ vs $\ln(1-x)$.

Formula S3:

The critical concentration distance (R_c) is estimated by the following expression:[3]

$$R_c = 2\left[\frac{3V}{4\Pi x_c Z}\right]^{1/3} \tag{S3}$$

where V, Z, and x_c represent the unit cell volume, the number of dopant effective sites in the unit cell, and the critical concentration of Eu^{3+} (V = 412.576 Å^3, Z = 4, and x_c = 0.5), respectively.

Formula S4:

To investigate the EM process between Eu^{3+} ions, the Dexter theory is employed:[4]

$$\frac{I}{x} = K[1 + \beta(x)^{\theta/3}]^{-1} \tag{S4}$$

where I and x represent the PL intensity and content of Eu^{3+} ions, respectively. K and β are constants. The type of electric multipolar interaction is reflected by the value of $\theta =$ 6, 8, and 10, corresponding to the dipole–dipole, dipole-quadrupole, and quadrupole-quadrupole, respectively.

Formula S5:

The external quantum efficiency (η_0), internal quantum efficiency (η_i), and absorption factor (α_{abs}) are calculated by the following formula:[5]

$$\eta_0 = \frac{\int L_S}{\int E_R}; \ \eta_i = \frac{\int L_S}{\int E_R - \int E_S}; \ \alpha_{abs} = \frac{\int E_R - \int E_S}{\int E_R} \tag{S5}$$

where L_S is the PL spectrum of the sample. E_R and E_S are the PLE spectra without and with the sample, respectively.

Formula S6:

CP can be estimated via the following equation:[6]

$$CP = \sqrt{(x - x_i)^2 + (y - y_i)^2} / \sqrt{(x_d - x_i)^2 + (y_d - y_i)^2} \tag{S6}$$

where x_i and y_i stand for the illuminant point (0.3101, 0.3162), which corresponds to the CIE 1931 Standard Source C. The color coordinates (x_d, y_d) come from the dominant emission.

Formula S7:

The activation energy (E_a) is evaluated by using the following expression:[7]

$$\ln(I_0/I - 1) = \ln A - E_a/kT \tag{S7}$$

where I_0 and I represent the integral intensities at room temperature and temperature T, respectively. k is the Boltzmann constant (8.62×10^{-5} eV/K), and A presents a coefficient.

Formula S8:

The Θ_D is evaluated by the following equation:[8]

$$(\Theta_D) = \sqrt{\frac{3h^2 T N_A}{A_i k U_{iso,i}}} \tag{S8}$$

where A_i is the atomic weight of the atom, h is the Planck constant, k is the Boltzmann constant, and $U_{iso,i}$ is the average atomic displacement parameter.

Formula S9:

The chromaticity shift (ΔE) is used to describe the chromaticity stability. It is calculated by the following formula:[9]

$$\Delta E = \sqrt{(u'_t - u'_0)^2 + (v'_t - v'_0)^2 + (w'_t - w'_0)^2} \tag{S9}$$

where $u' = 4x/(3 - 2x + 12y)$, $v' = 9y/(3 - 2x + 12y)$, and $w' = 1 - u' - v'$.

0 and t represent room temperature and given temperature, separately.

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