Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Modulating A site compositions of europium(III)-doped double-perovskite niobate phosphors

Yongbin Hua[a], Tian Wang[a], Jae Su Yu[a,*], Weiguang Ran[b,*], and Li Li[c,*]

[a]*Department of Electronics and Information Convergence Engineering, Institute for Wearable Convergence Electronics, Kyung Hee University, Yongin-si, Gyeonggi-do 17104, Republic of Korea.*

[b]*Department of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, P. R. China.*

[c]*School of Science, Chongqing University of Posts and Telecommunications, Chongqing 400065, P. R. China*

Table of contents of the supporting information.

Table S1. Rietveld refinement results of optimal samples.

	CINO:0.35Eu^{3+}	**SINO:0.1Eu^{3+}**	**BINO:0.3Eu^{3+}**
Radiation		Cu Kα_1 radiation	
Structure	Monoclinic	Monoclinic	Cubic
	(P21/n (14))	(P21/n (14))	(F m-3 m (225))
	a_1 = 5.550 Å	a_2 = 5.757 Å	a_3 = 8.343 Å
	b_1 = 5.760 Å	b_2 = 5.764 Å	b_3 = 8.343 Å
	c_1 = 7.989 Å	c_2 = 8.147 Å	c_3 = 8.343 Å
Lattice	α_1 = 90.0000º	α_2 = 90.0000º	α_3 = 90.0000º
parameters	β_1 = 90.0555º	β_2 = 89.9411º	β_3 = 90.0000º
	γ_1 = 90.0000º	γ_2 = 90.0000º	γ_3 = 90.0000º
	$V_1 \approx$ 255.392 Å^3	$V_2 \approx$ 270.345 Å^3	$V_3 \approx$ 580.720 Å^3

Table S2. Crystallographic data of the CINO:0.35Eu^{3+} phosphor.

Name	Fractional coordinates			Occ.	Site
Ca	0.507745	0.051501	0.260241	1	4e
In/Eu	0.000000	0.000000	0.000000	1	2a
Nb	0.000000	0.000000	0.500000	1	2b
O(1)	0.491853	0.954205	0.793617	1	4e
O(2)	0.128308	0.307279	1.056621	1	4e
O(3)	0.110920	-0.19688	0.256516	1	4e

Table S3. Crystallographic data of the SINO:0.1Eu^{3+} phosphor.

Name	Fractional coordinates			Occ.	Site
Sr	0.504600	-0.021400	0.248600	1	4e
In/Eu	0.000000	0.000000	0.000000	1	2a
Nb	0.500000	0.500000	0.000000	1	2b
O(1)	0.287900	0.775700	0.966300	1	4e
O(2)	0.224300	0.287900	0.966300	1	4e

O(3)	0.067400	0.013400	0.260600	1	4e

Table S4. Crystallographic data of the BINO:0.3Eu^{3+} phosphor.

Name	Fractional coordinates			Occ.	Site
Ba	0.250000	0.250000	0.250000	1	8c
In/Eu	0.000000	0.000000	0.000000	1	4a
Nb	0.500000	0.000000	0.000000	1	4b
O	0.261857	0.000000	0.000000	1	24e

Table S5. In-O distance in the [InO_6] octahedral.

	CINO	SINO	BINO
In-O(1)	2.144 Å	2.112 Å	
In-O(2)	2.170 Å	2.112 Å	2.094 Å
In-O(3)	2.150 Å	2.150 Å	

Table S6. O-In-O angle in the [InO_6] octahedral.

	CINO	SINO	BINO
O(1)-In-O(2)	89.56º	90.90º	
O(1)-In-O(3)	91.76º	90.50º	90.00º
O(2)-In-O(3)	87.68º	90.60º	

Table S7. Calculated lifetime results of CINO:0.35Eu^{3+} phosphor as a function of temperature.

T (K)	R^2	A_1	τ_1 (ms)	A_2	τ_2 (ms)	Average τ (ms)*
318	0.99988	16814.0373	0.5433	16814.0373	0.5433	0.543
338	0.99987	16926.12197	0.54225	16926.12197	0.54225	0.542
358	0.99989	16920.02447	0.5412	16920.02447	0.5412	0.541
378	0.9999	16879.47728	0.54089	16879.47728	0.54089	0.541
398	0.99992	16832.08815	0.54078	16832.08815	0.54078	0.541
418	0.9999	16768.08506	0.53915	16768.08506	0.53915	0.539
438	0.9999	16784.49744	0.53795	16784.49744	0.53795	0.538
458	0.9999	16780.78139	0.53745	16780.78139	0.53745	0.539
478	0.9999	16770.85855	0.53434	16770.85855	0.53434	0.534
498	0.99992	16651.56823	0.53332	16651.56823	0.53332	0.533
518	0.99992	30401.54064	0.52645	183.31514	1.23392	0.536
538	0.9999	63.42827	1.69871	26810.50767	0.52484	0.534
558	0.99988	19616.78506	0.49788	3126.23586	0.63912	0.522
578	0.99989	638.08585	0.77912	19467.04084	0.4938	0.508
598	0.99984	16951.02106	0.48776	1171.56358	0.25001	0.480

***Round to the nearest thousandth.**

Table S8. Calculated lifetime results of SINO:0.1Eu^{3+} phosphor as a function of temperature.

T (K)	R^2	A_1	τ_1 (ms)	A_2	τ_2 (ms)	Average τ (ms)*
318	0.9984	304.0131	1.09559	1713.71073	2.98917	2.87
338	0.99836	498.64467	1.54197	1494.81201	3.08165	2.86
358	0.99847	1531.75946	2.98206	457.95365	1.50258	2.79
378	0.99845	482.9848	1.47554	1518.18704	2.95444	2.75
398	0.99862	1661.07802	2.80419	317.51698	1.15729	2.68
418	0.99853	1575.99006	2.79875	441.68337	1.3473	2.63
438	0.99861	1508.65165	2.79352	522.72066	1.33096	2.59
458	0.9985	1709.1536	2.59044	313.74674	0.8482	2.49
478	0.99847	1586.3114	2.59439	406.71471	0.96549	2.45
498	0.99846	472.71421	0.91513	1569.8152	2.51839	2.36
518	0.99859	404.99643	0.67349	1650.57819	2.39332	2.28
538	0.99859	1575.79455	2.37846	452.8022	0.73722	2.24
558	0.99835	1507.49928	2.28598	413.20036	0.57086	2.18
578	0.99832	1539.76225	2.26478	456.73926	0.53641	2.15
598	0.99835	421.33094	0.51177	1546.10749	2.20871	2.11

***Round to the nearest hundredth.**

Table S9. Calculated lifetime results of BINO:0.3Eu^{3+} phosphor as a function of temperature.

T (K)	R^2	A_1	τ_1 (ms)	A_2	τ_2 (ms)	Average τ (ms)*
318	0.99842	7291.77525	1.65356	26504.94716	0.13657	1.30
338	0.99809	26877.52186	0.12423	6984.93082	1.5929	1.25
358	0.99763	6685.06103	1.50942	27598.15858	0.1078	1.19
378	0.99642	27875.27556	0.09469	6582.22505	1.40793	1.12
398	0.99526	6304.85194	1.33196	28373.4434	0.08518	1.05
418	0.9942	6129.25329	1.29662	28626.50801	0.08141	1.02
438	0.99255	28933.73566	0.07517	6053.69541	1.243	0.98
458	0.99175	6136.03345	1.17847	29542.68034	0.06918	0.93
478	0.99141	29916.9381	0.06611	6101.48707	1.12973	0.89
498	0.99048	6157.04395	1.0731	30537.81115	0.06167	0.85
518	0.98947	6186.80397	0.99483	32010.73315	0.05477	0.79
538	0.98879	6231.19757	0.93132	32840.38335	0.05107	0.73
558	0.98754	34565.5331	0.04599	6129.90678	0.85608	0.67
578	0.98702	6255.28308	0.77036	37288.74676	0.03983	0.60
598	0.98723	6335.48196	0.68706	40188.03512	0.0352	0.53

***Round to the nearest hundredth.**

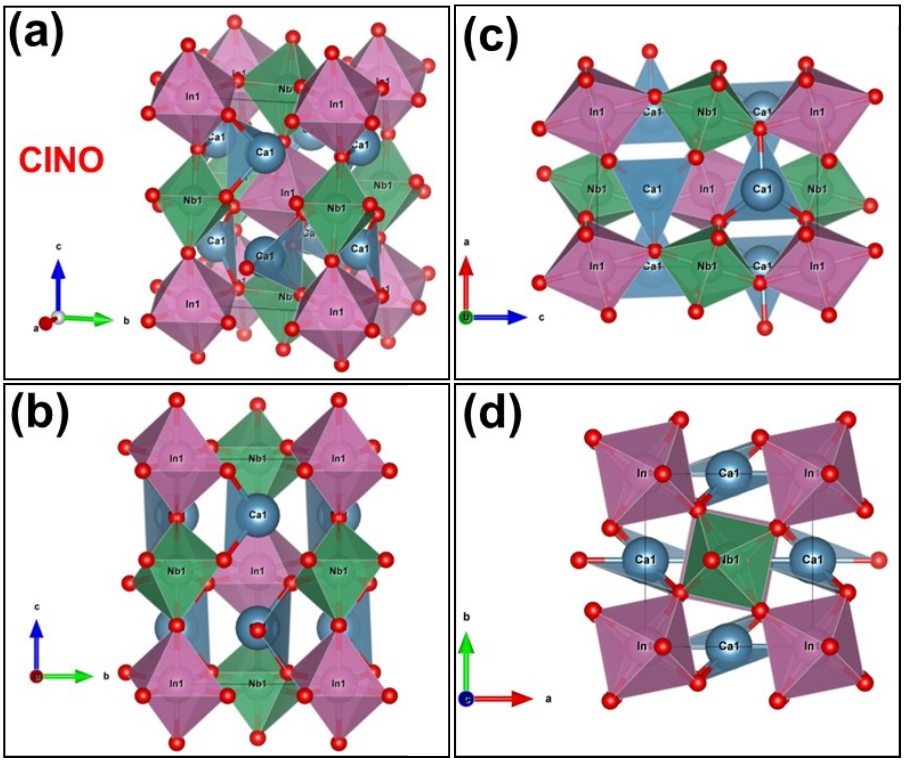

Fig. S1 (a-d) Crystal structure of the CINO material.

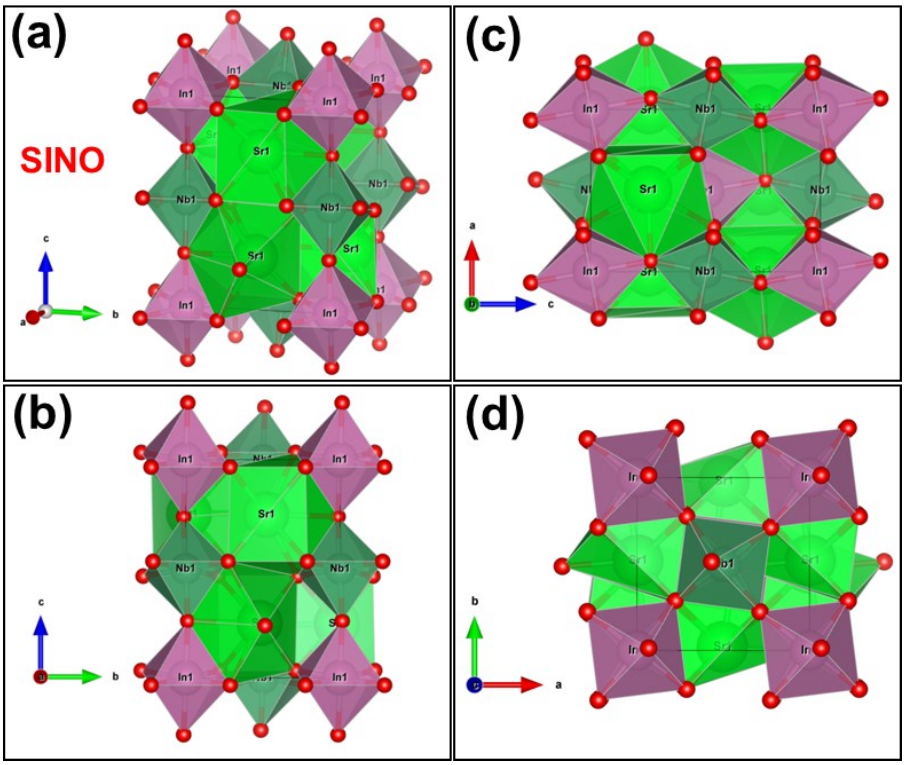

Fig. S2 (a-d) Crystal structure of the SINO material

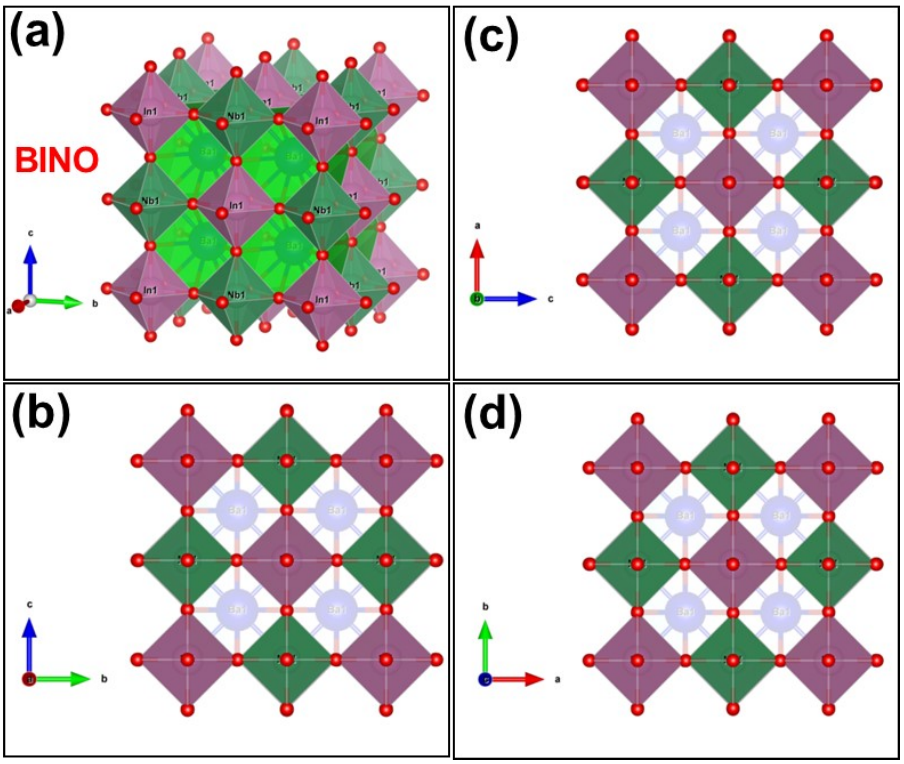

Fig. S3 (a-d) Crystal structure of the BINO material.

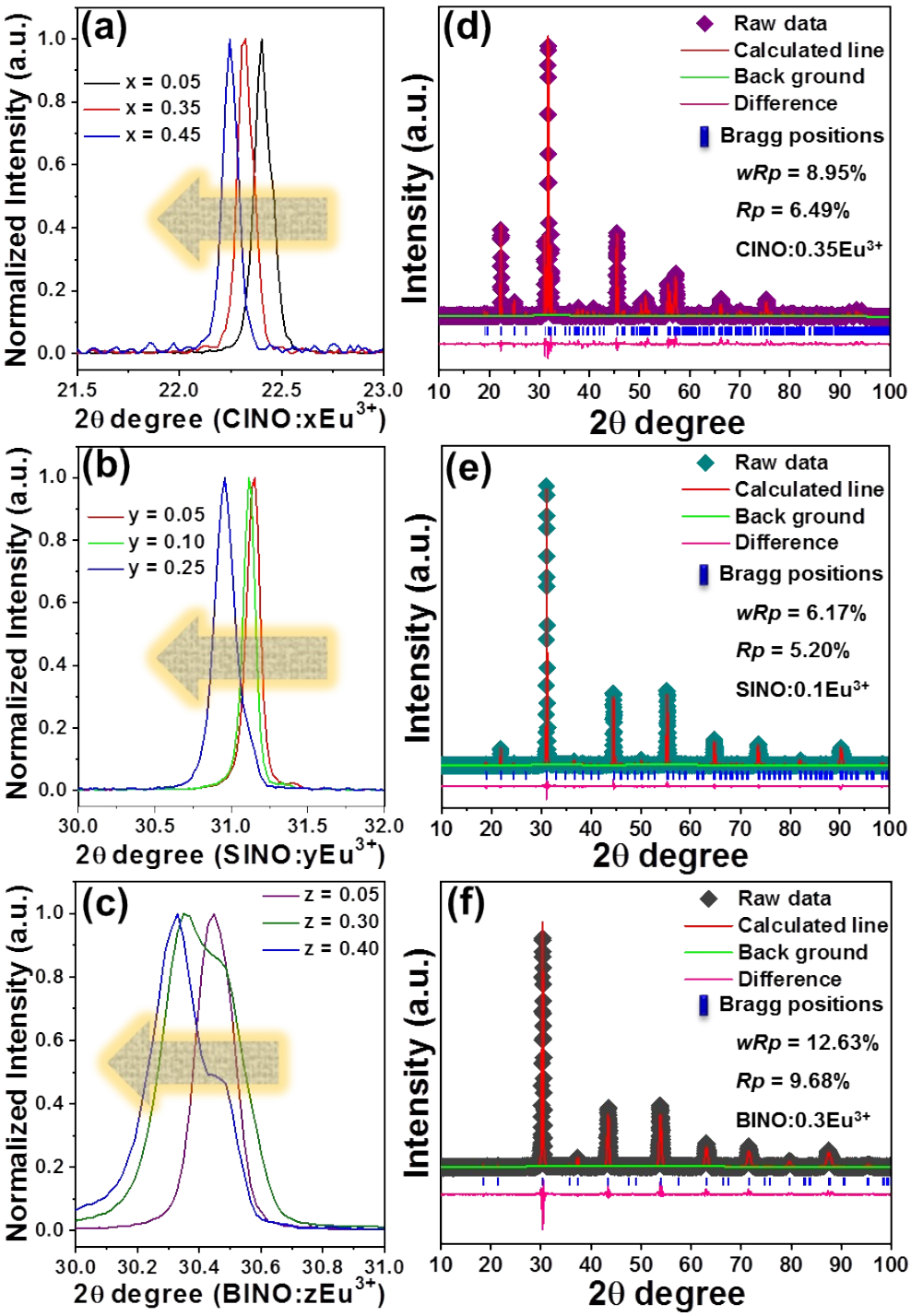

Fig. S4 Zoomed XRD patterns of the (a) CINO:xEu^{3+}, (b) SINO:yEu^{3+}, and (c) BINO:zEu^{3+} phosphors. Rietveld XRD refinements of (d) CINO:0.35Eu^{3+}, (e) SINO:0.1Eu^{3+}, and BINO:0.3Eu^{3+} phosphors.

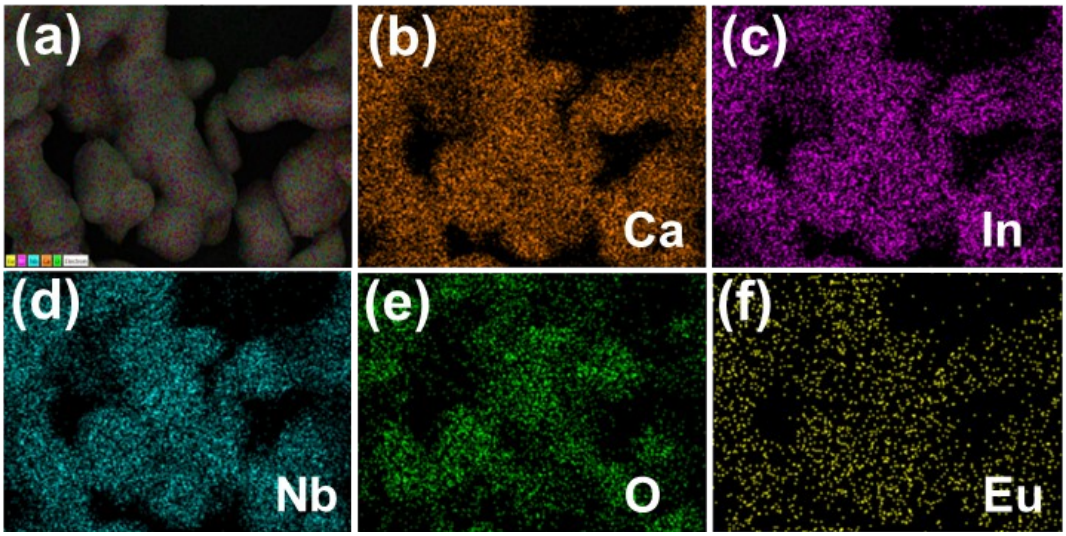

Fig. S5 (a-f) Elemental mappings of the CINO:0.1Eu^{3+} phosphor.

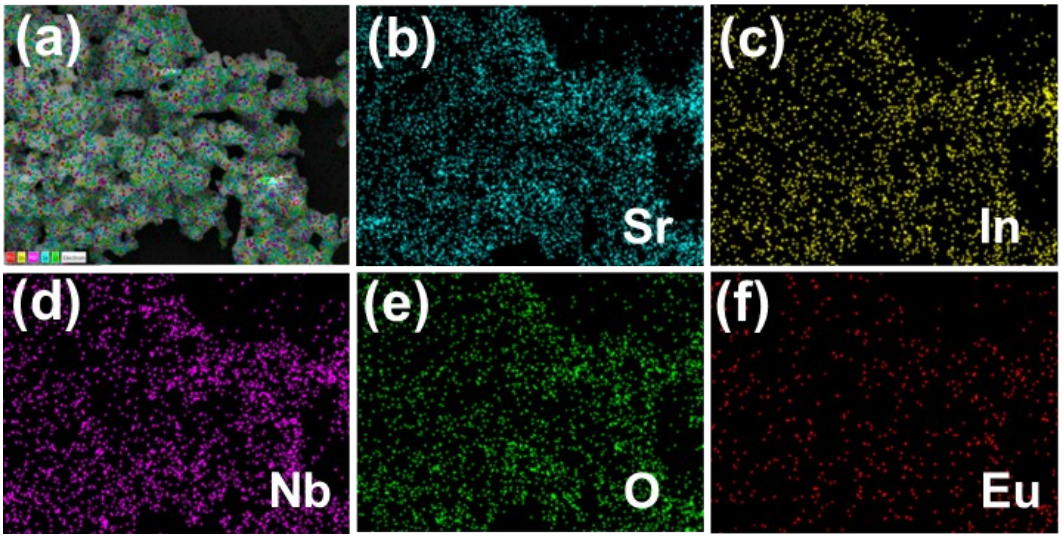

Fig. S6 (a-f) Elemental mappings of the SINO:0.1Eu^{3+} phosphor.

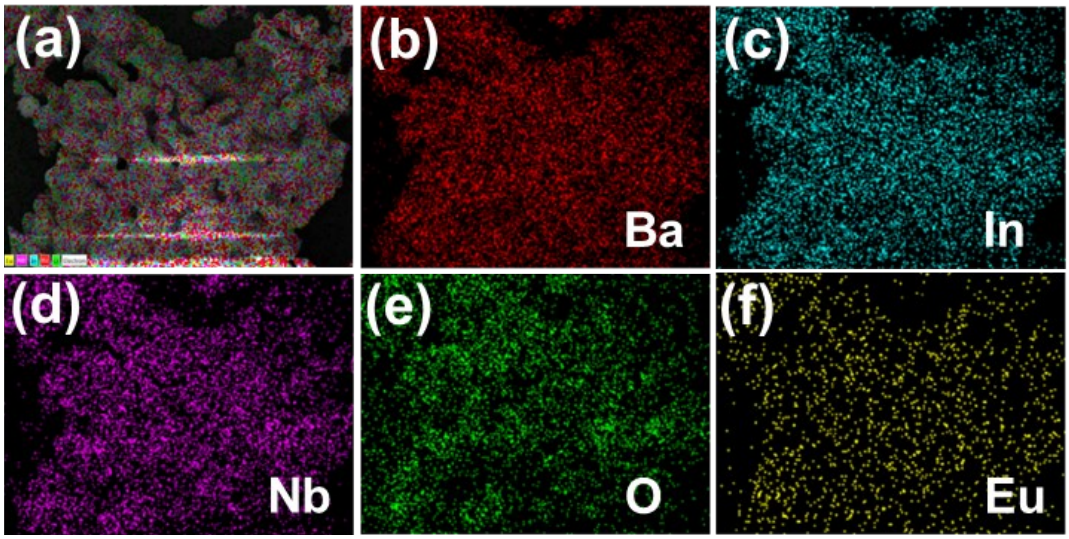

Fig. S7 (a-f) Elemental mappings of the BINO:0.1Eu^{3+} phosphor.

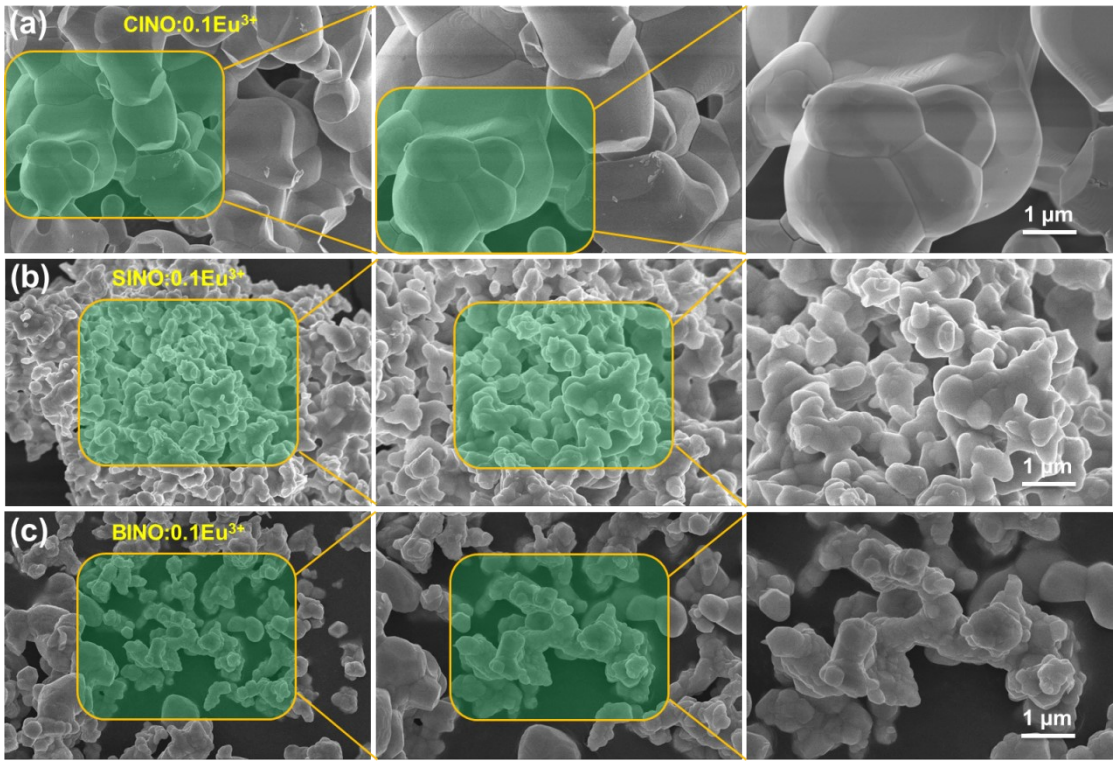

Fig. S8 FE-SEM images of the typical (a) CINO:0.1Eu^{3+}, (b) SINO:0.1Eu^{3+}, and (c) BINO:0.1Eu^{3+} phosphors under various magnifications.

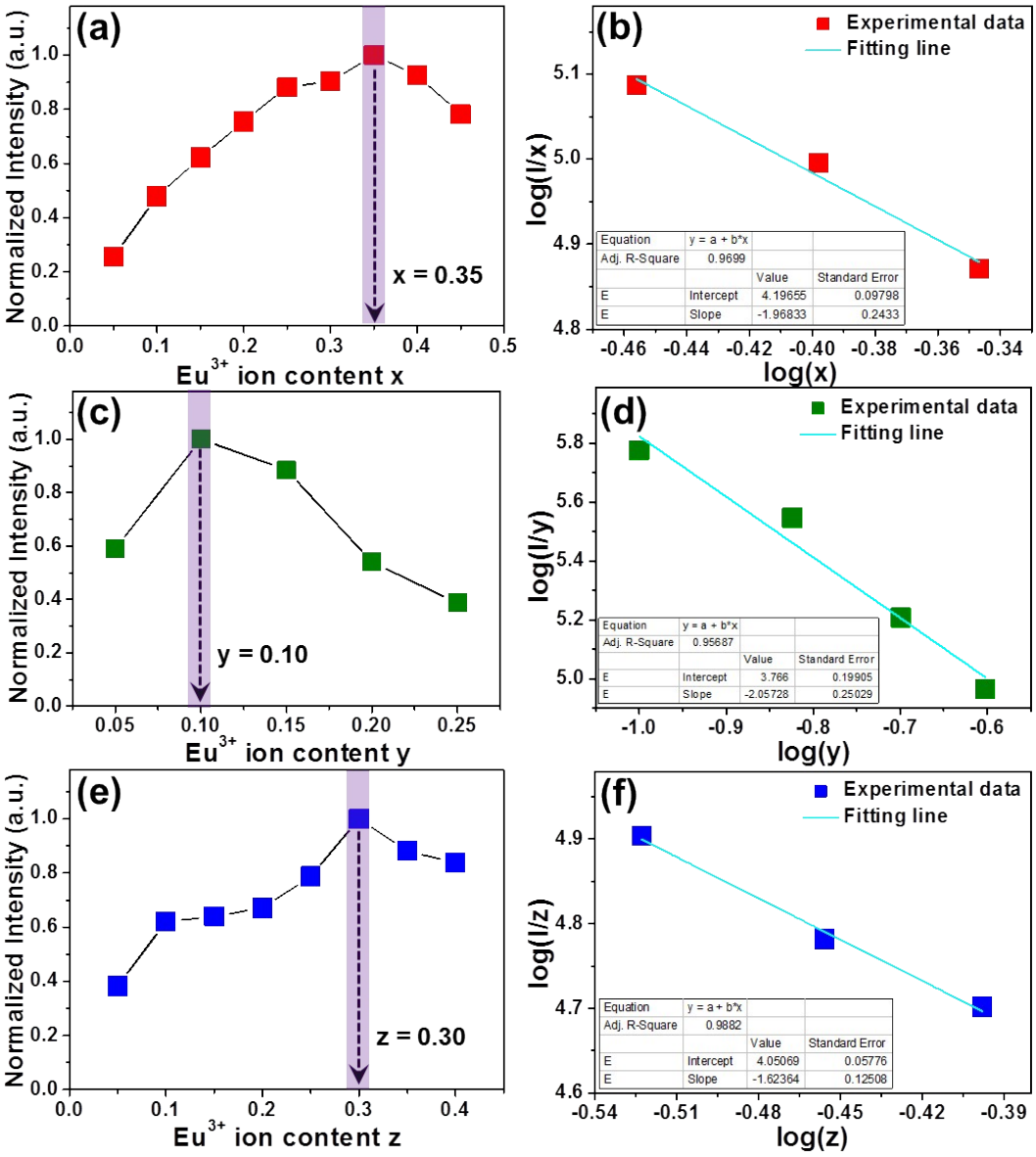

Fig. S9 Normalized emission intensity and plot of log(doping concentration) *vs.* log (emission intensity/doping concentration) of (a,b) CINO:xEu^{3+}, (c,d) SINO:yEu^{3+}, and (e,f) BINO:zEu^{3+} phosphors.

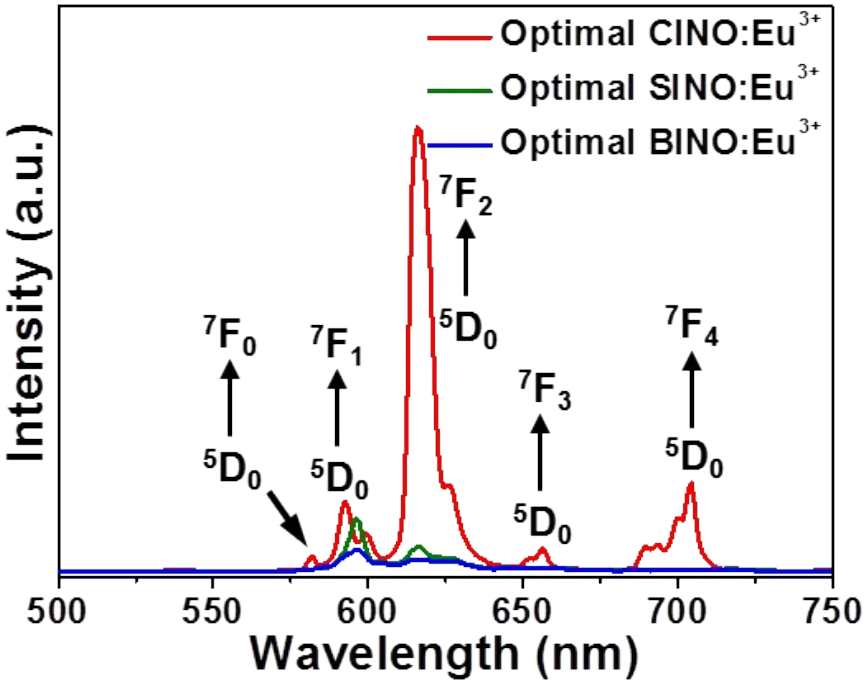

Fig. S10 PL emission spectra of the optimal resultant samples under same testing conditions.

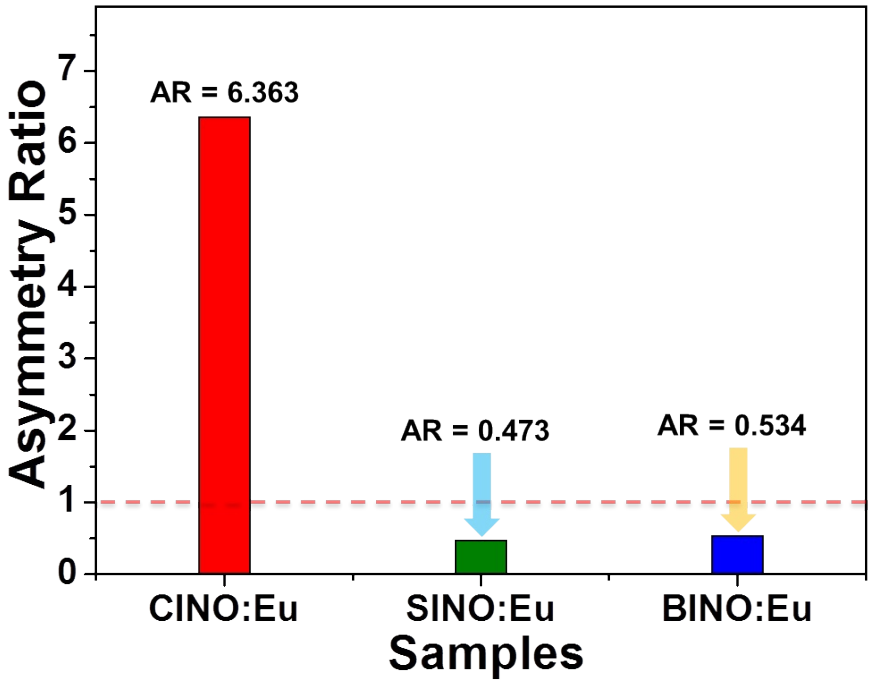

Fig. S11 Asymmetry ratio of the optimal resultant samples.

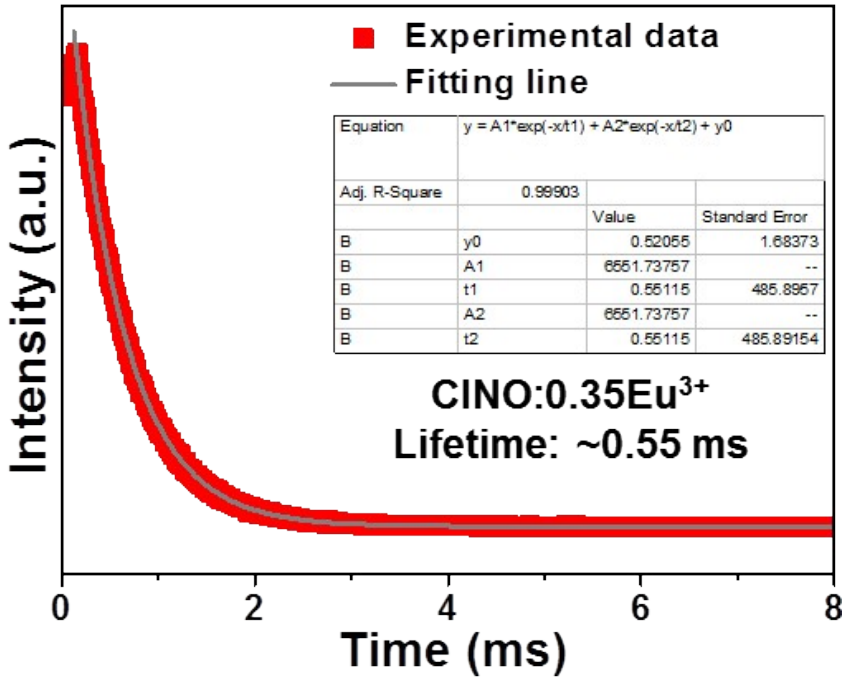

Fig. S12 Decay curve of the CINO:0.35Eu^{3+} phosphor.

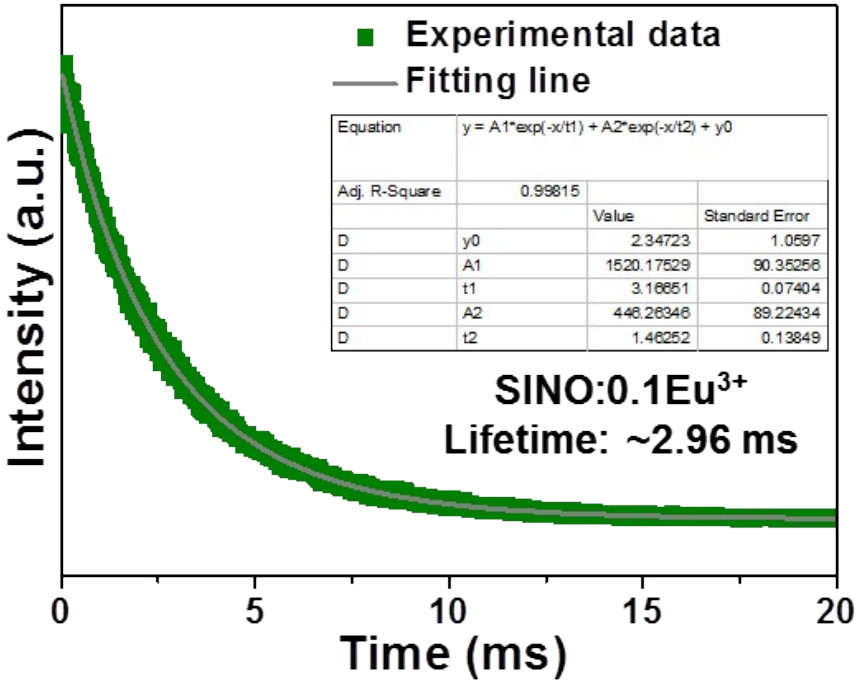

Fig. S13 Decay curve of the SINO:0.1Eu^{3+} phosphor.

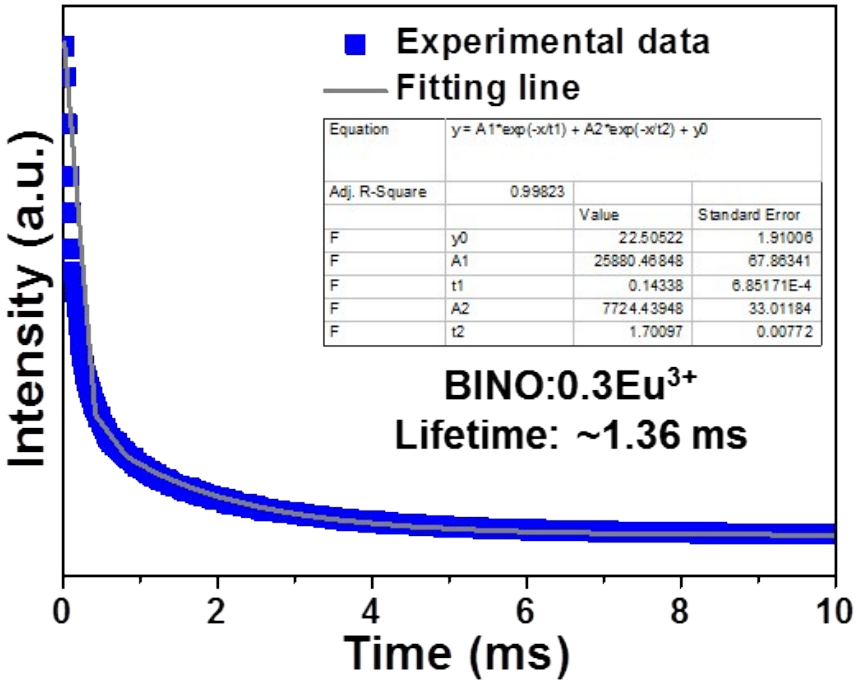

Fig. S14 Decay curve of the BINO:0.3Eu^{3+} phosphor.

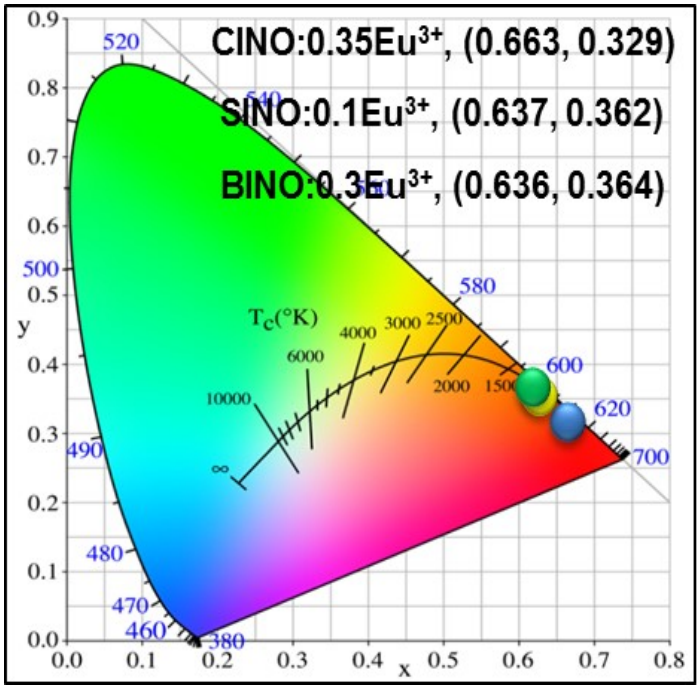

Fig. S15 Chromaticity coordinates of the optimal resultant samples.

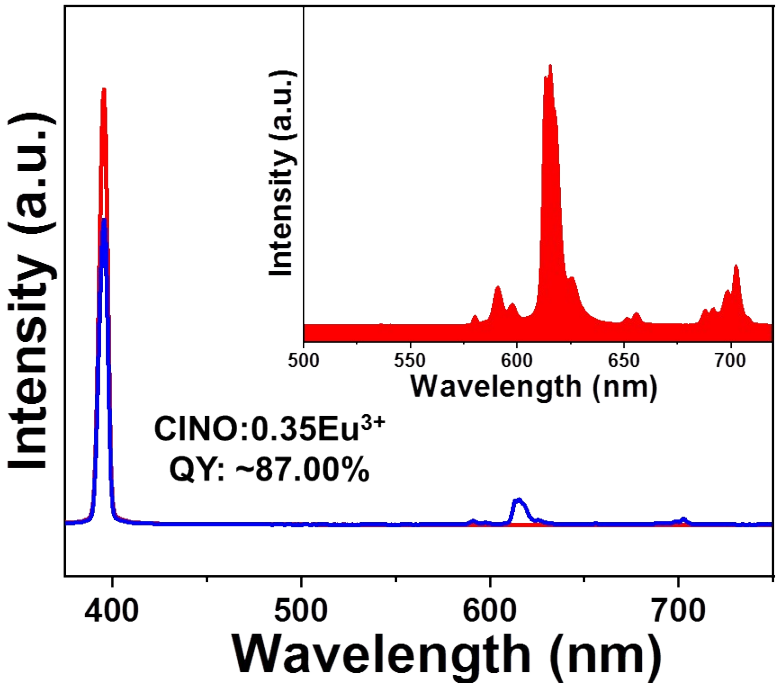

Fig. S16 Quantum yield pattern of the CINO:0.1Eu^{3+} phosphor.

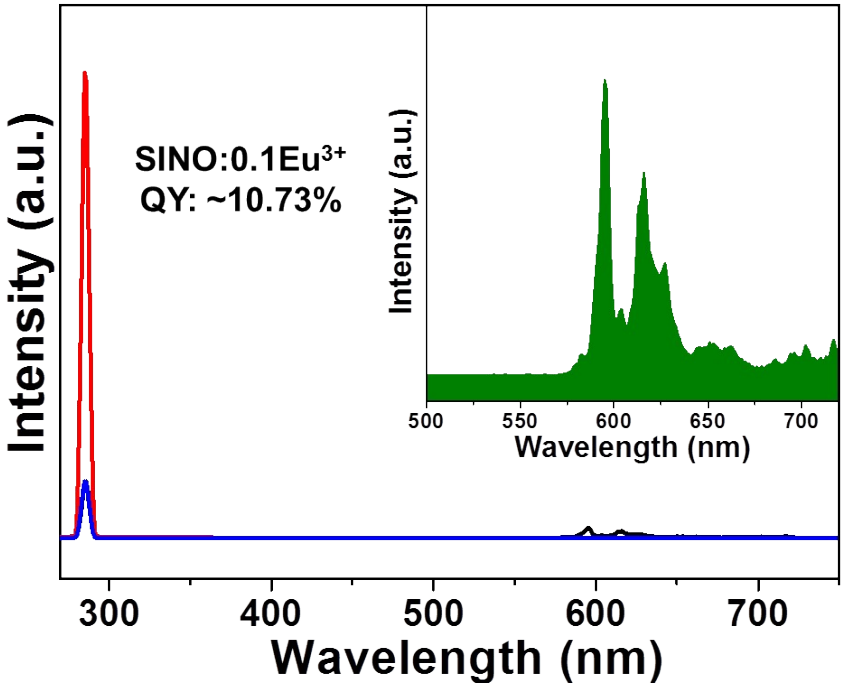

Fig. S17 Quantum yield pattern of the SINO:0.1Eu^{3+} phosphor.

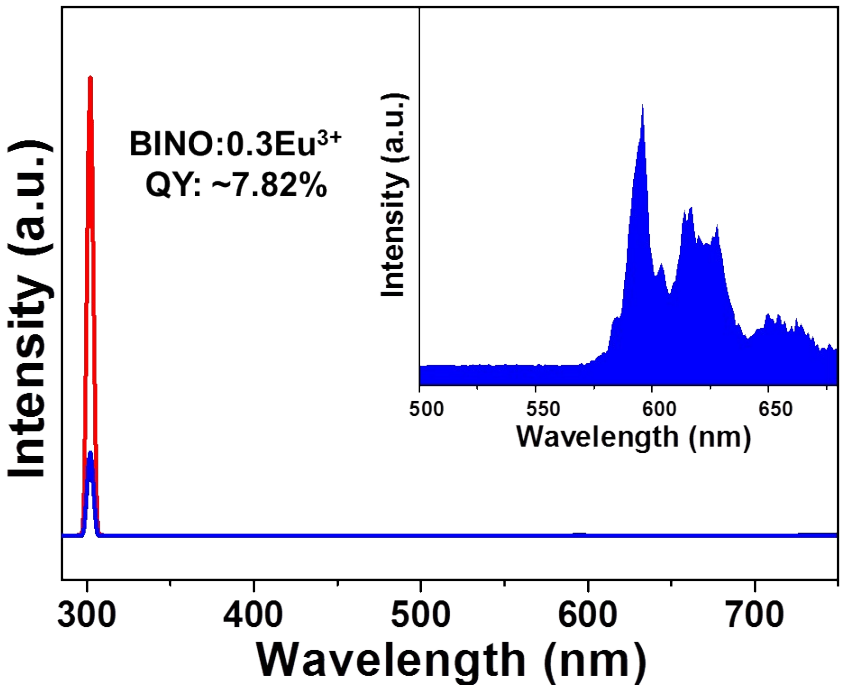

Fig. S18 Quantum yield pattern of the BINO:0.3Eu^{3+} phosphor.

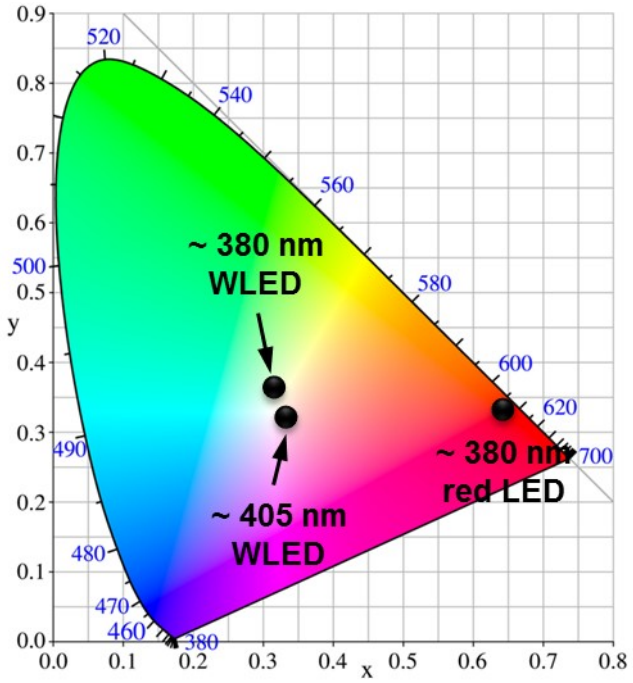

Fig. S19 Chromaticity coordinates of the packaged LED devices under the forward current of 300 mA.