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Supporting Information

Design of Broadband Near-Infrared $Y_{0.57}La_{0.72}Sc_{2.71}(BO_3)_4:Cr^{3+}$ Phosphors Based on One-Site Occupation and Its Application in NIR Light-Emitting Diodes

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Computational details

The calculations were carried out using density functional theory with the PBE.[1] The Vienna ab-initio simulation package (VASP)[2-5] was employed. The plane wave energy cutoff was set as 400 eV. The Fermi scheme was employed for electron occupancy with an energy smearing of 0.1 eV. The first Brillouin zone was sampled in the Monkhorst−Pack grid.[6,7] The energy (converged to 1.0 $\times 10^{-6}$ eV/atom) and force (converged to 0.01eV/Å) were set as the convergence criterion for geometry optimization. The spin polarization was considered in all calculation. For Cr, the Coulomb interaction corrections with Hubbard-like U term of 3 eV are also considered for 3d.

Table S1 Rietveld fitting results of YLSBO and YLSBO:0.025Cr^{3+}

formula	YLSBO	YLSBO:0.025Cr^{3+}
crystal system	trigonal	trigonal
space group	*R*32	*R*32
a (Å)	9.8048(6)	9.7993(8)
b (Å)	9.8048(6)	9.7993(8)
c (Å)	8.0101(6)	7.9919(7)
$\alpha = \beta$(deg)	90	90
γ (deg)	120	120
Z	3	3
V (Å^3)	666.87(10)	664.62(13)
R_p	0.0638	0.0593
R_{wp}	0.0862	0.0785
χ^2	5.928	8.806

Table S2 Atomic positions of YLSBO

atom	site	x	y	z	occupancy	U_{iso}
Y1	3a	0	0	0	0.28	0.02126
Y2	9d	-0.1219	0.6667	0.6667	0.1	0.00955
La1	3a	0	0	0	0.72	0.02126
Sc1	9d	-0.1219	0.6667	0.6667	0.9	0.00955
B1	9e	-0.2212	0.6667	0.1667	1.000	0.00128
B2	3b	0	0	0.5	1.000	0.00102
O1	9e	0	-0.4091	0.5	1.000	0.00509
O2	18f	-0.0114	0.2029	-0.1997	1.000	0.03002
O3	9e	0	-0.1386	0.5	1.000	0.01100

Table S3 Atomic positions of YLSBO:0.025Cr^{3+}

atom	site	x	y	z	occupancy	U_{iso}
Y1	3a	0	0	0	0.28	0.02682
Y2	9d	-0.1209	0.6667	0.6667	0.1	0.00799
La1	3a	0	0	0	0.72	0.02682
Sc1	9d	-0.1209	0.6667	0.6667	0.875	0.00799
Cr1	9d	-0.1209	0.6667	0.6667	0.025	0.00799
B1	9e	-0.2212	0.6667	0.1667	1.000	0.05884
B2	3b	0	0	0.5	1.000	0.06022
O1	9e	0	-0.4074	0.5	1.000	0.01351
O2	18f	-0.0104	0.2103	-0.2081	1.000	0.04746
O3	9e	0	-0.1363	0.5	1.000	0.03537

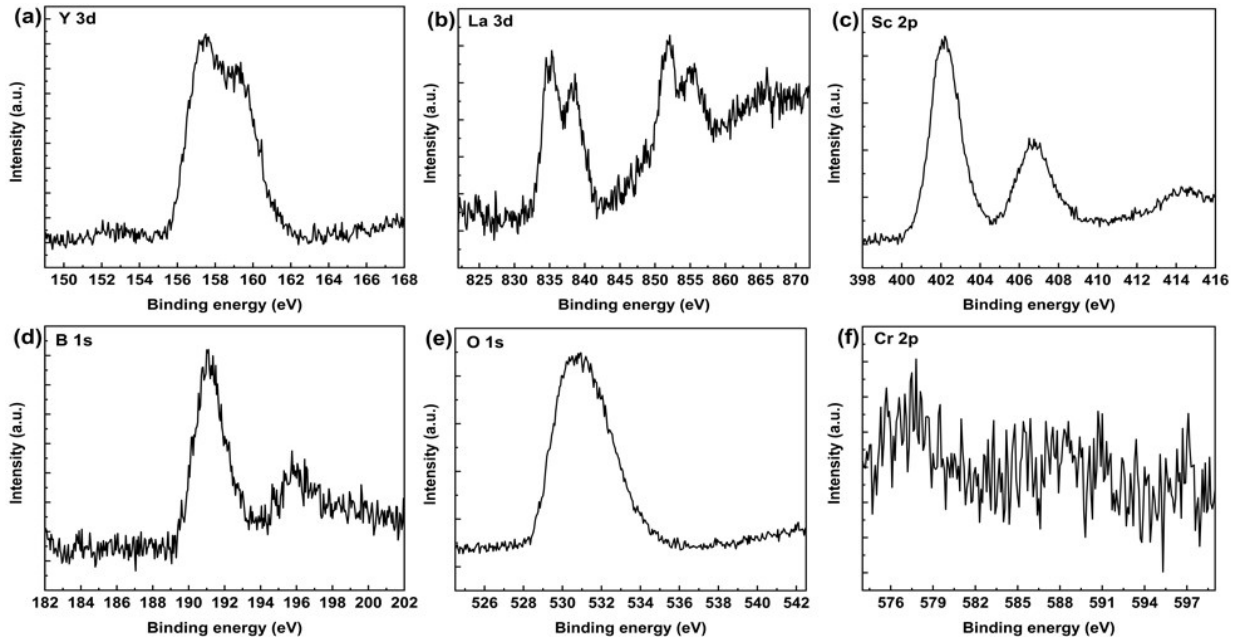

Fig. S1 (a−f) Y 3d, La 3d, Sc 2p, B 1s, O 1s and Cr 2p XPS of $Y_{0.57}La_{0.72}Sc_{2.71}(BO_3)_4$:0.025$Cr^{3+}$ sample.

Table S4 Luminescent paramaters of Cr^{3+} in different host materials

phosphor	$\lambda_{em\ (nm)}$	FWHM	PL range (nm)	ref
YLSBO:0.025Cr^{3+}	850	172	650–1200	this work
$Ca_2LuZr_2Al_3O_{12}$:0.08Cr^{3+}	750	117	700–850	8
$La_3Sc_2Ga_3O_{12}$:0.01Cr^{3+}	818	145	700–1100	9
$NaScSi_2O_6$:0.06Cr^{3+}	840	140	750–950	10
$La_3GaGe_5O_{16}$:0.07Cr^{3+}	780	160	650–1050	11
$Ca_2LuHf_2Al_3O_{12}$:0.08Cr^{3+}	780	145	700–1100	12

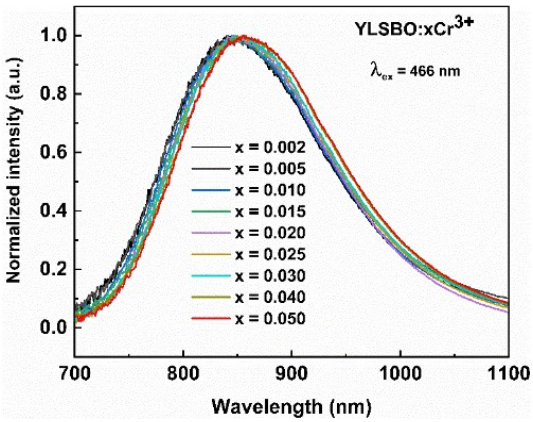

Fig. S2 The normalized PL emission spectra of the YLSBO:xCr^{3+} (x = 0.002, 0.005, 0.01,0.015, 0.02, 0.025, 0.03, 0.04, and 0.05) phosphors (λ_{ex} = 466 nm).

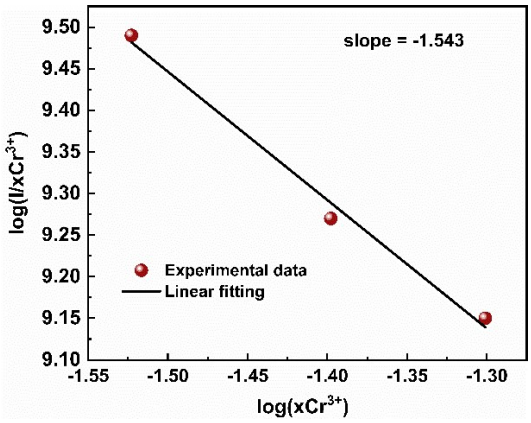

Fig. S3 Relationship of log(I/xCr^{3+}) with log(xCr^{3+}) in YLSBO:xCr^{3+} (x = 0.03, 0.04, and 0.05) phosphors (λ_{ex} = 466 nm).

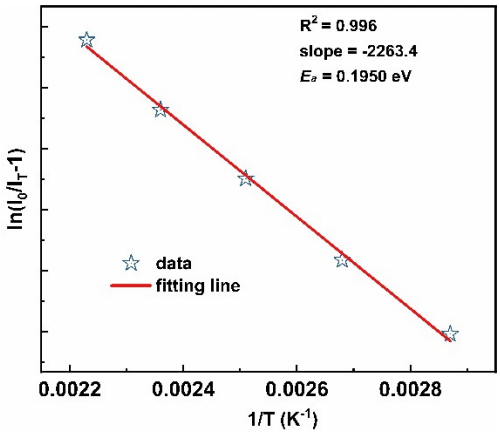

Fig. S4 The relationship of ln[(I_0/I_T)−1] with 1/T in YLSBO:xCr^{3+} phosphor.

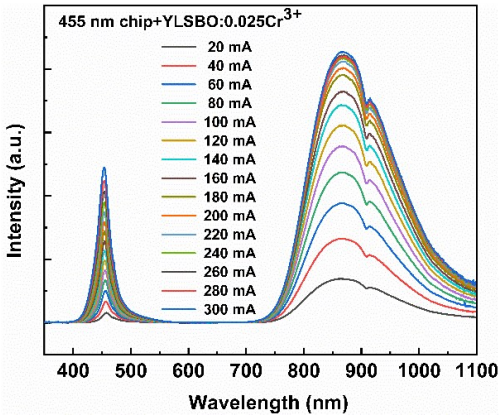

Fig. S5 PL spectra of the NIR pc-LED at various driving currents.

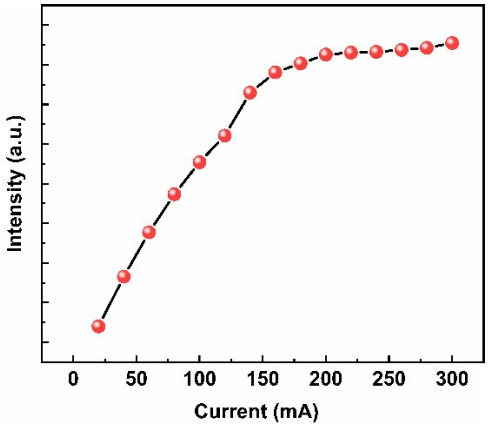

Fig. S6 The corresponding PL intensities as a function of driving current.

Table S5 The properties of NIR-LEDs prepared using YLSBO:0.025Cr^{3+} phosphor.

Current (mA)	Voltage (V)	Input power (mW)	Output power (mW)
20	2.643	52.60	2.616
40	2.720	108.5	5.033
60	2.782	166.6	7.176
80	2.836	226.6	9.064
100	2.884	287.8	10.69
120	2.928	351.1	12.06
140	2.969	415.4	13.31
160	3.008	481.0	14.27
180	3.047	548.1	15.31
200	3.082	616.1	15.90
220	3.116	685.3	16.42
240	3.149	755.5	16.76
260	3.182	827.1	17.11
280	3.214	899.5	17.18
300	3.247	973.9	17.61

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