

Supporting Information

A Novel Dy³⁺-Activated Single-Phase White Light-Emitting Phosphor for Solid-State Lighting

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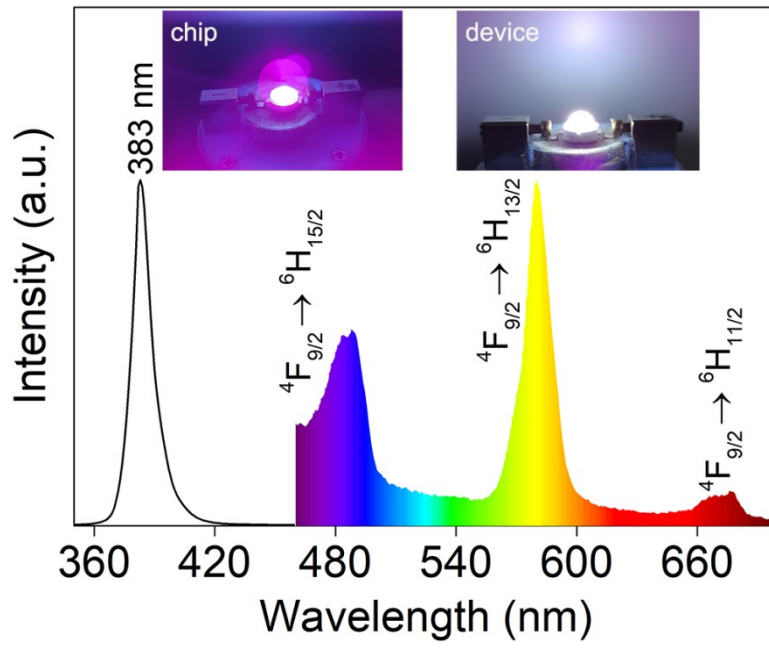


Fig. S1 Electroluminescence spectrum of SCB:0.03Dy³⁺ phosphor-based LED device.

Table S1 The Sc-O and Ca-O bond lengths of SCB: $x\text{Dy}^{3+}$

SCB:0.03 Dy^{3+}		SCB:0.07 Dy^{3+}		SCB:0.11 Dy^{3+}	
Sc/Dy-O	Ca-O	Sc/Dy-O	Ca-O	Sc/Dy-O	Ca-O
2.2679 (37)	2.2966 (31)	2.1833 (57)	2.2327 (65)	2.1549 (43)	2.2884 (44)
2.1692 (51)	2.4098 (38)	2.2928 (44)	2.4032 (39)	2.3024 (54)	2.8346 (87)
2.2679 (37)	2.7715 (67)	2.2928 (44)	2.2942 (37)	2.1945 (68)	2.3038 (80)
2.0989 (27)	2.3605 (56)	2.1137 (63)	2.7863 (77)	2.3024 (54)	2.2884 (87)
2.1027 (55)	2.4098 (38)	2.1097 (29)	2.3312 (66)	2.1549 (43)	2.4236 (47)
2.0989 (27)	2.2966 (31)	2.1097 (29)	2.2942 (37)	2.1842 (75)	2.1462 (76)
	2.2527 (56)		2.4032 (39)		2.4236 (47)

Table S2 The refined structure parameters of SCB:0.03Dy³⁺.

Phosphor	Atom	Wyck.	x/a	y/b	z/c	Occ.	U (Å ²)
	Sc(Dy)	4c	0.3883	1.25	0.5725	1.0000	0.018
	Ca	4c	0.5885	3/4	0.8388	1.0000	0.004
	B1	4c	0.3120	1.25	0.8697	1.0000	0.020
SCB:0.03Dy ³⁺	O1	4c	0.5036	3/4	0.6178	1.0000	0.014
	O2	4c	0.2413	1.25	0.7393	1.0000	0.003
	O3	4c	0.2595	3/4	0.4916	1.0000	0.019
	O4	4c	0.4379	1/4	0.8682	1.0000	0.020

Space group: Pnma (62) - orthorhombic.

Cell parameters: a = 10.1820 Å, b = 3.3742 Å, c = 9.4137 Å.

V = 323.41 Å³, Z = 4.

Reliability factors: $R_p = 6.80\%$, $wR_p = 8.97\%$.

Table S3 The refined structure parameters of SCB:0.07Dy³⁺.

Phosphor	Atom	Wyck.	x/a	y/b	z/c	Occ.	U (Å ²)
	Sc(Dy)	4c	0.3891	1.25	0.5731	1.000	0.025
	Ca	4c	0.5886	3/4	0.8394	1.000	0.001
	B1	4c	0.3103	1.25	0.8716	1.000	0.026
SCB:0.07Dy ³⁺	O1	4c	0.5052	3/4	0.6201	1.000	0.024
	O2	4c	0.2397	1.25	0.7395	1.000	0.005
	O3	4c	0.2566	3/4	0.4923	1.000	0.030
	O4	4c	0.4383	1/4	0.8661	1.000	0.034.

Space group: Pnma (62) - orthorhombic.

Cell parameters: a = 10.1801 Å, b = 3.3812 Å, c = 9.4154 Å.

$V = 324.09 \text{ Å}^3$, $Z = 4$.

Reliability factors: $R_p = 6.33\%$, $wR_p = 8.04\%$.

Table S4 The refined structure parameters of SCB:0.11Dy³⁺.

Phosphor	Atom	Wyck.	x/a	y/b	z/c	Occ.	U (Å ²)
	Sc(Dy)	4c	0.3880	1.25	0.5735	1.000	0.032
	Ca	4c	0.5877	3/4	0.8404	1.000	-0.002
	B1	4c	0.3178	1.25	0.8830	1.000	0.018
SCB:0.11Dy ³⁺	O1	4c	0.5082	3/4	0.6294	1.000	0.049
	O2	4c	0.2397	3/4	0.4937	1.000	0.008
	O3	4c	0.2538	3/4	0.4937	1.000	0.035
	O4	4c	0.4377	1/4	0.8599	1.000	0.038

Space group: Pnma (62) - orthorhombic.

Cell parameters: a = 10.1923 Å, b = 3.3856 Å, c = 9.4187 Å.

$V = 325.01 \text{ Å}^3$, $Z = 4$.

Reliability factors: $R_p = 5.97\%$, $wR_p = 8.06\%$.