

Supporting information

Aliovalent Substitution Toward Reinforced Structural Rigidity in Ce³⁺-Doped Garnet Phosphors Featuring Improved Performance

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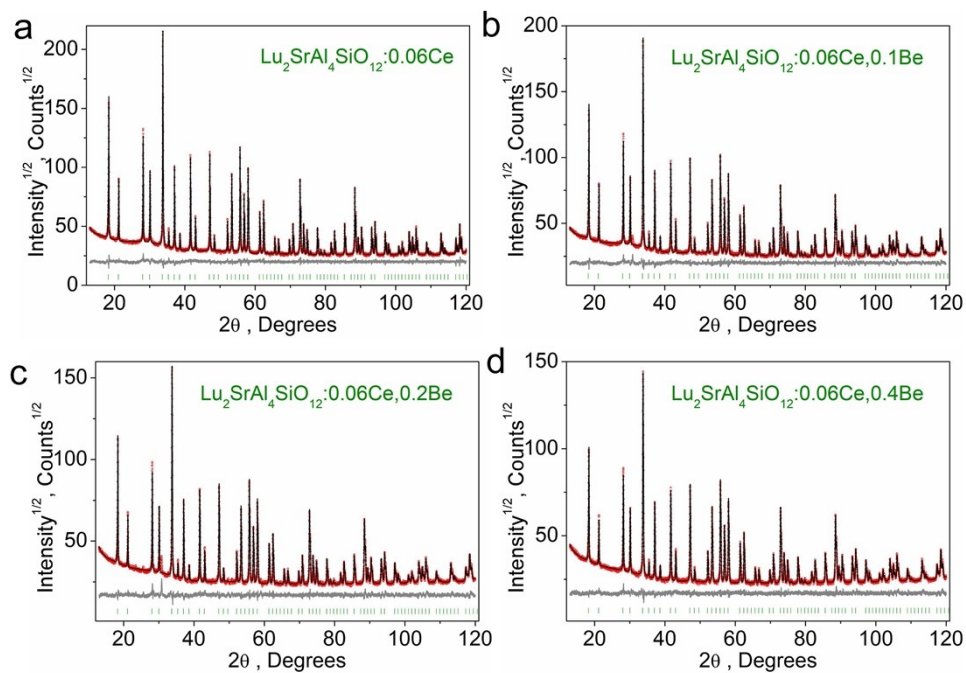


Figure S1. Difference Rietveld plot of $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}:0.06\text{Ce}, x\text{Be}$ ($x=0, 0.1, 0.2,$ and 0.4) compounds.

Table S1. Main parameters of processing and refinement of the $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}:0.06\text{Ce}, x\text{Be}$.

x	0	0.1	0.2	0.4
Sp.Gr.	<i>Ia-3d</i>	<i>Ia-3d</i>	<i>Ia-3d</i>	<i>Ia-3d</i>
a , Å	11.91513 (5)	11.90465 (4)	11.89969 (8)	11.89585 (11)
V , Å ³	1691.59 (2)	1687.13 (2)	1685.03 (3)	1683.40 (5)
Z	8	8	8	8
2θ -interval, °	13-120	13-120	13-120	13-120
R_{wp} , %	4.68	4.99	5.41	4.66
R_p , %	3.63	3.91	4.03	3.64
R_{exp} , %	2.80	2.92	3.16	3.29
χ^2	1.67	1.71	1.71	1.42
R_B , %	2.08	2.19	2.25	1.78

Table S2. Fractional atomic coordinates and isotropic displacement parameters (\AA^2) of $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}$: 0.06Ce , $x\text{Be}$

	<i>x</i>	<i>y</i>	<i>z</i>	B_{iso}	Occ.
<i>x</i> = 0					
Lu	1/4	1/8	0	0.27 (3)	0.6566667
Sr	1/4	1/8	0	0.27 (3)	0.3233333
Ce	1/4	1/8	0	0.27 (3)	0.02
Al1	0	0	0	1.35 (5)	1
Al2	1/4	3/8	0	1.59 (5)	2/3
Si2	1/4	3/8	0	1.59 (5)	1/3
O	0.03129 (19)	0.05267 (18)	0.64933 (16)	1.15 (7)	1
<i>x</i> = 0.1					
Lu	1/4	1/8	0	0.20 (4)	0.6566667
Sr	1/4	1/8	0	0.20 (4)	0.3233333
Ce	1/4	1/8	0	0.20 (4)	0.02
Al1	0	0	0	1.36 (6)	1
Al2	1/4	3/8	0	1.47 (5)	0.645
Si2	1/4	3/8	0	1.47 (5)	0.322
Be2	1/4	3/8	0	1.47 (5)	0.033
O	0.0321 (2)	0.0526 (2)	0.64971 (18)	1.27 (7)	1
<i>x</i> = 0.2					
Lu	1/4	1/8	0	0.20 (3)	0.6566667
Sr	1/4	1/8	0	0.20 (3)	0.3233333
Ce	1/4	1/8	0	0.20 (3)	0.02
Al1	0	0	0	1.30 (6)	1
Al2	1/4	3/8	0	1.18 (5)	0.622
Si2	1/4	3/8	0	1.18 (5)	0.311
Be2	1/4	3/8	0	1.18 (5)	0.067
O	0.0323 (2)	0.0521 (2)	0.6502 (2)	1.34 (8)	1
<i>x</i> = 0.4					
Lu	0.25	0.125	0	0.20 (3)	0.6566667
Sr	0.25	0.125	0	0.20 (3)	0.3233333

Ce	0.25	0.125	0	0.20 (3)	0.02
Al1	0	0	0	1.22 (5)	1
Al2	0.25	0.375	0	0.80 (4)	0.578
Si2	0.25	0.375	0	0.80 (4)	0.289
Be2	0.25	0.375	0	0.80 (4)	0.133
O	0.0317 (2)	0.0515 (2)	0.65107 (19)	1.48 (7)	1

Table S3. Main bond lengths (Å) of Lu₂SrAl₄SiO₁₂: 0.06Ce, xBe

x = 0			
(Lu/Sr/Ce)—O ⁱ	2.398 (2)	Al1—O ⁱⁱⁱ	1.923 (2)
(Lu/Sr/Ce)—O ⁱⁱ	2.302 (2)	(Al2/Si2)—O ^{iv}	1.755 (2)
x = 0.1			
(Lu/Sr/Ce)—O ⁱ	2.399 (2)	Al1—O ⁱⁱⁱ	1.927 (2)
(Lu/Sr/Ce)—O ⁱⁱ	2.306 (2)	(Al2/Si2/Be2)—O ^{iv}	1.744 (2)
x = 0.2			
(Lu/Sr/Ce)—O ⁱ	2.405 (2)	Al1—O ⁱⁱⁱ	1.931 (2)
(Lu/Sr/Ce)—O ⁱⁱ	2.302 (2)	(Al2/Si2/Be2)—O ^{iv}	1.735 (2)
x = 0.4			
(Lu/Sr/Ce)—O ⁱ	2.411 (2)	Al1—O ⁱⁱⁱ	1.936 (2)
(Lu/Sr/Ce)—O ⁱⁱ	2.288 (2)	(Al2/Si2/Be2)—O ^{iv}	1.730 (2)

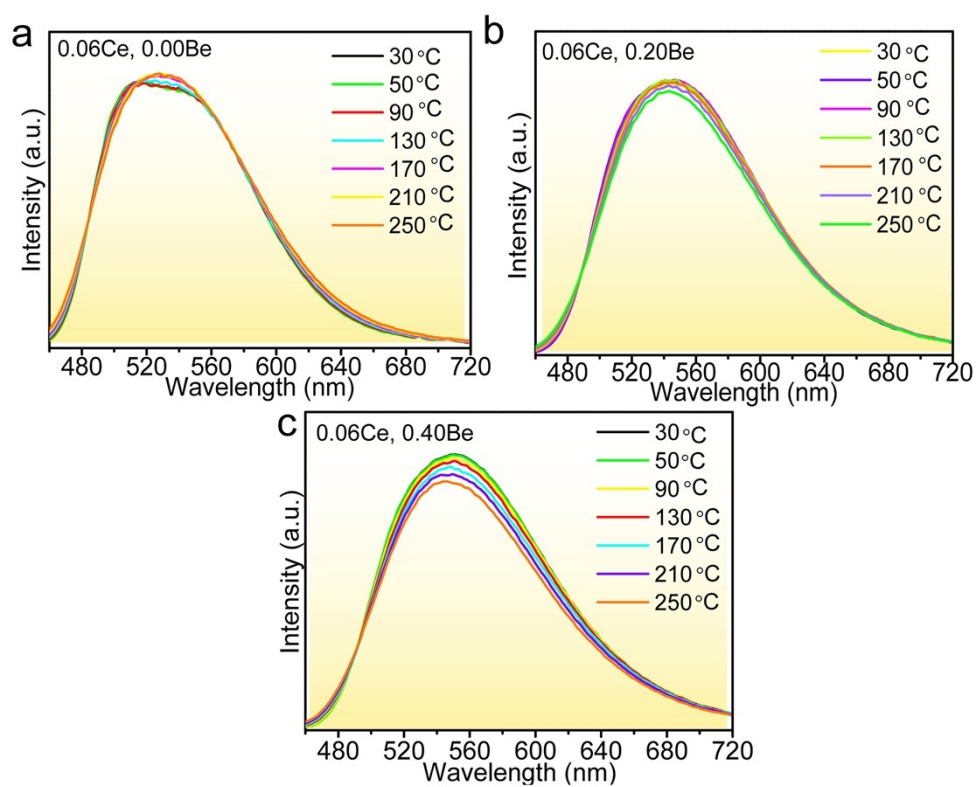
Symmetry codes: (i) -x+1/4, -z+3/4, y-1/4; (ii) -z+1, -x, -y; (iii) -x, y, z-1/2; (iv) z-1/2, -x+1/2, -y; (v) -y+1/2, z-1/2, x.

Table S4. Quantum efficiencies of three representative Lu₂SrAl₄SiO₁₂:0.06Ce, xBe phosphors.

Samples	IOE(%)	Abs.	EQE(%)
x = 0.00	79.2	0.337	26.69
x = 0.20	82.2	0.377	30.99
x = 0.40	84.5	0.39	32.95

Table S5. CIE coordinate data of $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}: 0.06\text{Ce}, x\text{Be}$.

Samples	CIE x	CIE y
$x = 0.00$	0.3086	0.5758
$x = 0.05$	0.3272	0.5800
$x = 0.10$	0.3439	0.5792
$x = 0.20$	0.3634	0.5742
$x = 0.30$	0.3802	0.5652
$x = 0.40$	0.3953	0.5611
$x = 0.50$	0.4110	0.5540

**Figure S2.** Emission spectra of $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}: 0.06\text{Ce}, x\text{Be}$ ($x = 0, 0.2$ and 0.4) phosphors in the temperature range of 30-250 °C.

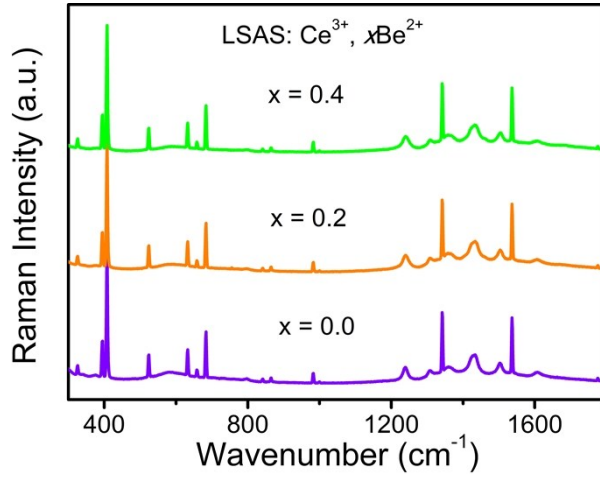


Figure S3. Raman spectra of $\text{Lu}_2\text{SrAl}_4\text{SiO}_{12}: 0.06\text{Ce}, x\text{Be}$ ($x = 0, 0.2$ and 0.4) phosphors.

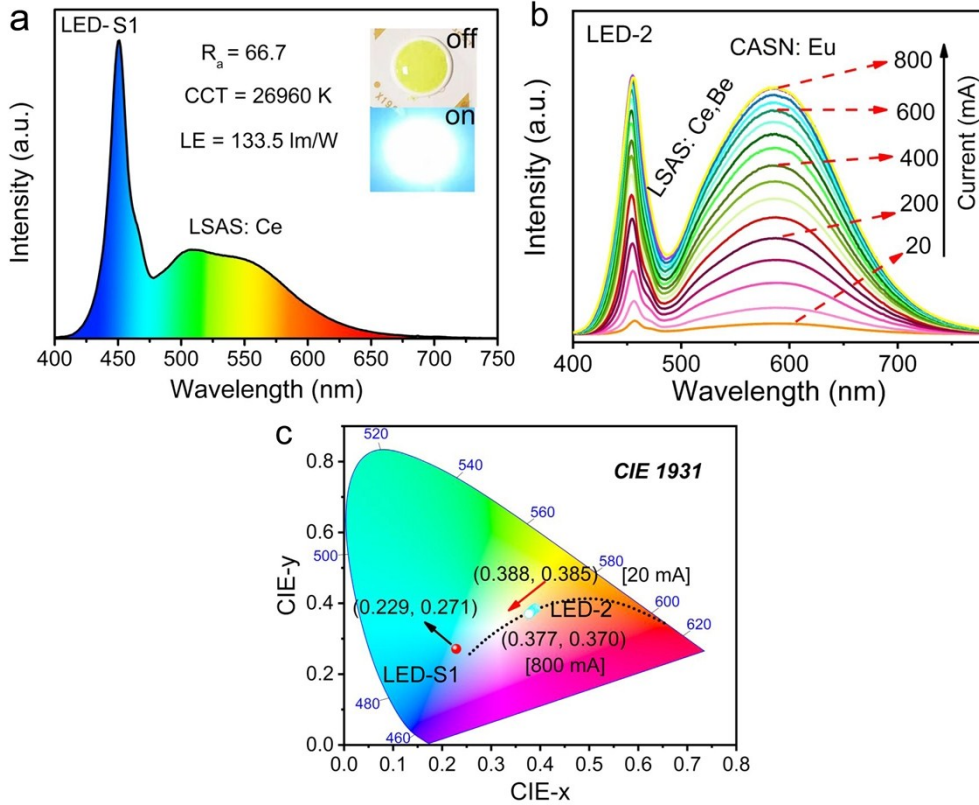


Figure S4. (a) Emission spectra of WLED devices fabricated by green LSAS: Ce phosphor. (b) Current-dependent emission spectra of LED-2 in the current range of 20-800 mA. (c) The CIE color coordinates of LED-S1 and the LED-2 at different currents.

Table S6. Luminous efficiencies of LED-2 driven at various currents

Currents/(mA)	LE/(lm/W)	Currents/(mA)	LE/(lm/W)
50	142.9	400	100.2
80	137.5	450	95.3
110	133.4	500	90.9
140	128.6	550	86.6
170	124.5	600	82.1
200	121.1	650	78.4
250	115.2	700	73.5
300	109.9	750	70.1
350	104.8	800	64.5
