Supporting information

Remarkable structure and luminescence regulation of $Gd_2LuAl_5O_{12}$:Ce garnet phosphor with Ca^{2+}/Si^{4+} pair for high-quality w-WLED lighting

Qinghong Meng,[a] Guoying Zhao,[b,c] Qi Zhu,[a] Xudong Sun,[a,d] Ji-Guang Li[c,*]

[a]*Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education) and School of Materials Science and Engineering, Northeastern University, Shenyang, Liaoning 110819, China*

[b]*School of Materials Science and Engineering, Shanghai Institute of Technology, Shanghai 201418, China*

[c]*Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan*

[d]*Foshan Graduate school of Northeastern University, Foshan, Guangdong 528311, China*

[*]Corresponding author

Dr. Ji-Guang Li

National Institute for Materials Science

Tel: +81-29-860-4394

E-mail: LI.Jiguang@nims.go.jp

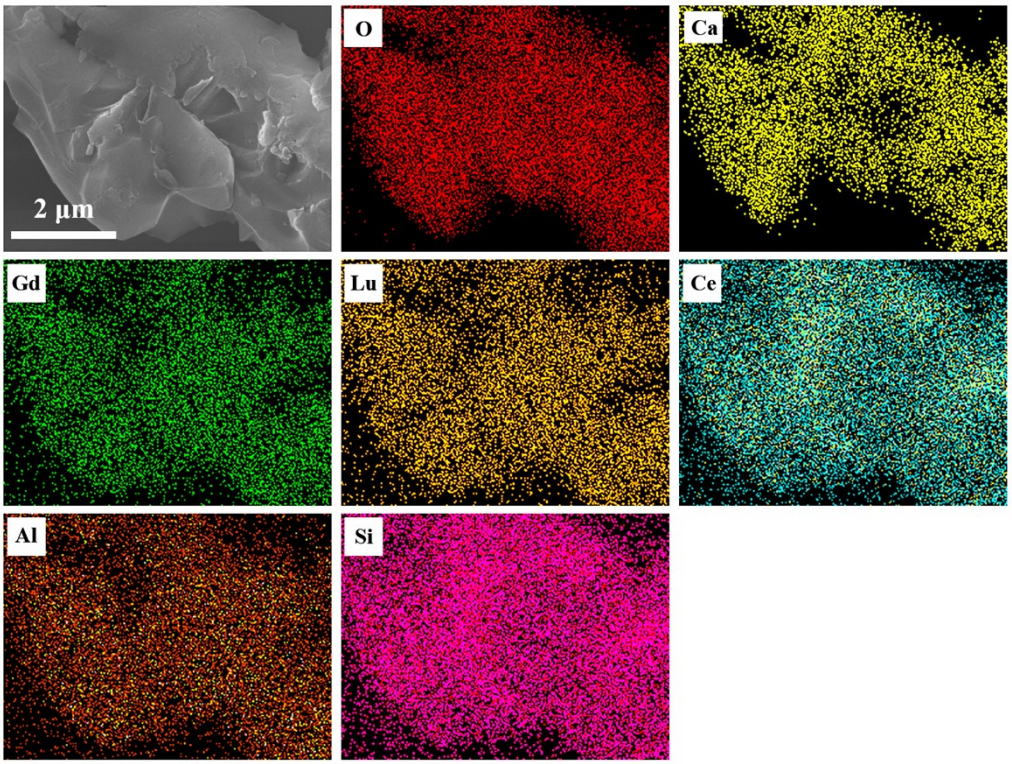

Fig. S1 The results of EDS mapping for the local aera shown by the FE-SEM micrograph of the $Gd_{0.77}LuCa_{1.2}Al_{3.8}Si_{1.2}O_{12}$ (x =1.2) garnet phosphor.

Table S1 Crystallographic data, atomic coordinates (x, y, z), atomic occupancy (Occ.) and isotropic displacement parameter (Å^2) for the typical $Gd_{1.97-x}LuCa_xAl_{5-x}Si_xO_{12}$:0.03Ce phosphors of x = 0.0, 0.6 and 1.2.

x=0.0	Atom	Position	x	y	z	Occ.	B_{iso}
$Gd_{1.97}LuAl_5O_{12}$:0.03Ce	Gd	24c	1/8	0	1/4	0.657	0.23(2)
a =b =c = 12.0484(9) Å	Lu	24c	1/8	0	1/4	0.333	0.23(2)
V = 1749.0(4) Å^3	Ce	24c	1/8	0	1/4	0.01	0.23(2)
R_{wp} = 12.43%	Al1	16a	0	0	0	1	0.06(9)
R_p = 8.64%	Al2	24d	3/8	0	1/4	1	0.14(7)
χ^2 = 1.28	O	96h	0.9697(3)	0.0476(3)	0.1497(3)	1	0.17(1)
x=0.6							
$Gd_{1.37}LuCa_{0.6}Al_{4.4}Si_{0.6}O_{12}$:0.03Ce	Gd	24c	1/8	0	1/4	0.457	0.48(3)
a =b =c = 12.0102(1) Å	Lu	24c	1/8	0	1/4	0.333	0.48(3)
V = 1732.4(4) Å^3	Ca	24c	1/8	0	1/4	0.20	0.48(3)
R_{wp} = 12.72%	Ce	24c	1/8	0	1/4	0.01	0.48(3)
R_p = 9.59%	Al1	16a	0	0	0	1	0.57(1)
χ^2 = 1.58	Al2	24d	3/8	0	1/4	0.80	0.54(8)
	Si	24d	3/8	0	1/4	0.20	0.54(8)
	O	96h	0.9669(3)	0.0477(4)	0.1496(3)	1	0.62(1)

x=1.2							
$Gd_{0.77}LuCa_{1.2}Al_{3.8}Si_{1.2}O_{12}$:0.03Ce	Gd	24c	1/8	0	1/4	0.257	0.16(2)
$a = b = c$ = 11.9754(7) Å	Lu	24c	1/8	0	1/4	0.333	0.16(2)
V = 1717.4(3) Å^3	Ca	24c	1/8	0	1/4	0.40	0.16(2)
R_{wp} = 8.92%	Ce	24c	1/8	0	1/4	0.01	0.16(2)
R_p = 6.75%	Al1	16a	0	0	0	1	0.63(5)
χ^2 = 1.85	Al2	24d	3/8	0	1/4	0.60	0.57(4)
	Si	24d	3/8	0	1/4	0.40	0.57(4)
	O	96h	0.9641(2)	0.0477(2)	0.1495(2)	1	0.94(7)

χ^2 was defined as R_{wp}/R_{exp} in the Users' Manual of TOPAS V4.2 software. R_p, R_{wp} and R_{exp} are pattern reliability factor, weighted profile reliability factor and expected reliability factor, respectively.

Table S2 The d_4, d_6, d_{82}, d_{84} and d_{av} bond distances for the typical $Gd_{1.97-x}LuCa_xAl_{5-x}Si_xO_{12}$:0.03Ce phosphors of x = 0.0, 0.6 and 1.2.

	d_4	d_6	d_{82}	d_{84}	d_{av}
x=0.0	1.7589(4)	1.9271(4)	2.3002(3)	2.4831(4)	2.3917
x=0.6	1.7319(4)	1.9274(4)	2.3211(4)	2.4798(5)	2.4005
x=1.2	1.7066(2)	1.9282(2)	2.3428(2)	2.4776(3)	2.4102

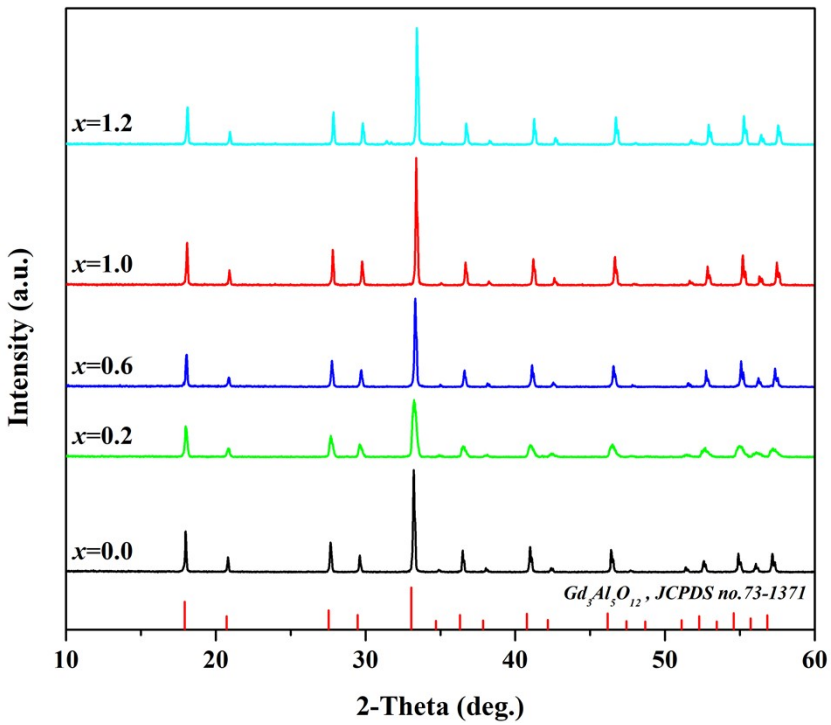

Fig. S2 XRD patterns of the $Gd_{2-x}LuCa_xAl_{5-x}Si_xO_{12}$ (GLCSAG, x = 0.0−1.2) garnet hosts, which revealed that they conform to the GLCSAG:Ce phosphor products shown in Fig. 1, respectively.