

Supporting information

Governing the Crystallographic Sites for Tuning Eu²⁺ Emission in an Apatite Oxyfluoride Host to be Applied for Superior White Light Emitting Diodes

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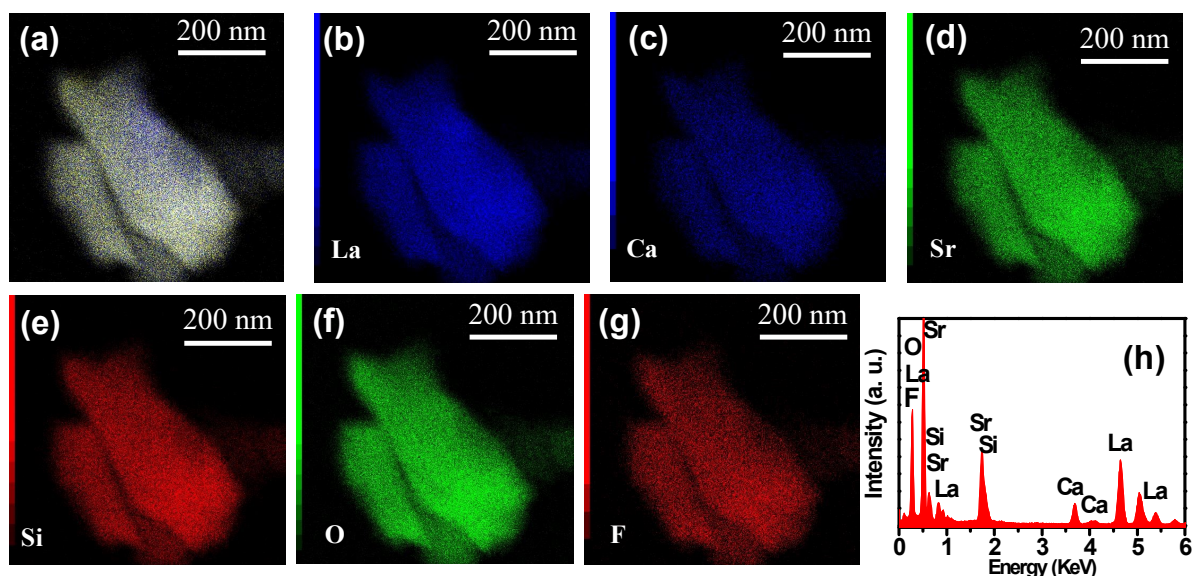


Fig. S1 (a) TEM spectrum, (b-g) elemental mapping images, and (h) EDX spectra of CSLOF.

Table S1 Rietveld refined lattice parameters of CLOF, CLOF: 0.04Eu²⁺, CSLOF, CSLOF: 0.04Eu²⁺ and CSLOF: 0.04Eu²⁺;1.2Ba²⁺.

Formula	CLOF	CLOF:0.04Eu ³⁺	CSLOF	CSLOF:0.04Eu ²⁺	CSLOF:0.04Eu ²⁺ ;1.2Ba ²⁺
Structure	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space group	P 63/m (# 176)	P 63/m (# 176)	P 63/m (# 176)	P 63/m (# 176)	P 63/m (# 176)
a = b [Å]	9.6553 (3)	9.6494 (5)	9.6855 (5)	9.6902 (4)	9.7247 (2)
c [Å]	7.1224 (1)	7.1202 (2)	7.1622 (8)	7.1649 (5)	7.2090 (3)
v [Å ³]	575.03 (1)	574.15 (6)	582.19 (7)	582.65 (1)	590.42 (3)
Z	2	2	2	2	2
χ ²	1.527	2.171	5.323	3.856	3.234
R _p (%)	3.76	4.94	5.57	6.02	5.44
R _{wp} (%)	4.98	6.59	9.13	8.58	8.67
GOF (S)	1.24	1.47	2.31	1.96	1.80
Temperature	298 K	298 K	298 K	298 K	298 K

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Table S2 The atomic coordinates and fractional occupancies of CLOF and CSLOF hosts

Atom	Wyck. pos.	x	y	z	U_{iso}	Occ.
CLOF						
La1	6h	0.23691 (3)	-0.01380	1/4	0.0176 (2)	0.75
Ca1	6h	0.23691 (3)	-0.01380	1/4	0.0176 (2)	0.25
La2	4f	2/3	1/3	0.00238 (9)	0.0046 (1)	0.375
Ca2	4f	2/3	1/3	0.00238 (9)	0.0046 (1)	0.625
Si	6h	0.39769 (4)	0.36628 (1)	1/4	0.0215 (4)	1.0
O1	6h	0.58661 (8)	0.47220 (4)	1/4	0.0249 (8)	1.0
O2	6h	0.33204 (5)	0.48359 (2)	1/4	0.0087 (4)	1.0
O3	12i	0.34109 (1)	0.26277 (4)	0.06359 (6)	0.0170 (8)	1.0
F	2a	0	0	1/4	0.1475 (2)	1.0
CSLOF						
La1	6h	0.24120 (6)	-0.01259 (3)	1/4	0.0199 (9)	0.75
Ca1	6h	0.24120 (6)	-0.01259 (3)	1/4	0.0199 (9)	0.125
Sr1	6h	0.24120 (6)	-0.01259 (3)	1/4	0.0199 (9)	0.125
La2	4f	2/3	1/3	0.00198 (3)	0.0057 (6)	0.375
Ca2	4f	2/3	1/3	0.00198 (3)	0.0057 (6)	0.3125
Sr2	4f	2/3	1/3	0.00198 (3)	0.0057 (6)	0.3125
Si	6h	0.39272 (5)	0.35948 (9)	1/4	0.0220 (5)	1.0
O1	6h	0.57470 (2)	0.45330 (2)	1/4	0.0463 (5)	1.0
O2	6h	0.33411 (1)	0.48183 (8)	1/4	0.0385 (4)	1.0
O3	12	0.34445 (9)	0.25447 (1)	0.05584 (6)	0.0196 (3)	1.0
F	2	0	0	1/4	0.0598 (8)	1.0