Supporting Information

Design of Mixed-Anionic-Ligands System for a Blue-Light-Excited Orange-Yellow Emission Phosphor $Ba_{1.31}Sr_{3.69}(BO_3)_3Cl:Eu^{2+}$

Haiyan Wu,[a,b] Huimin Li,[c] Lihong Jiang,*[a] Ran Pang,[a] Su Zhang,[a] Da Li,[a] Guanyu Liu,[a] Chengyu Li,*[a,b] Jing Feng[a] and Hongjie Zhang[a]

a. State Key Laboratory of Rare Earth Resource Utilization Changchun Institute of Applied Chemistry Chinese Academy of Sciences Changchun 130022, China

b. University of Science and Technology of China Hefei 230026, China

c. Engineering Product Development Singapore University of Technology and Design 8 Somapah Road, Singapore 487372, Singapore

* *Corresponding author: Tel.:+86-0431-85262258*

E-mail address: cyli@ciac.ac.cn and lhjiang@ciac.ac.cn

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 Eu, the Coulomb interaction corrections with Hubbard-like U term of 6 eV are also considered for 4f.

Table S1 Rietveld fitting results of BSBOC:0.025Eu^{2+}

formula	BSBOC:0.025Eu^{2+}
crystal system	orthorhombic
space group	*Pnma*
a (Å)	6.9368(3)
b (Å)	16.4567(8)
c (Å)	9.5281(5)
$\alpha = \beta = \gamma$ (deg)	90
Z	4
V (Å^3)	1087.70(11)
R_p	0.0528
R_{wp}	0.0730
χ^2	3.744

Table S2 Atomic positions of BSBOC:0.025Eu^{2+}

atom	site	x	y	z	Occupancy	U_{iso}
Ba1	8d	0.3615	0.4104	0.1114	0.6550	0.0135
Sr1	8d	0.3615	0.4104	0.1114	0.3416	0.0135
Sr2	8d	0.4964	0.3998	0.7194	0.9892	0.0096
Sr3	4c	0.4759	0.2500	0.4694	0.9892	0.0110
Eu1	8d	0.3615	0.4104	0.1114	0.0034	0.0135
Eu2	8d	0.4964	0.3998	0.7194	0.0108	0.0096
Eu3	4c	0.4759	0.2500	0.4694	0.0108	0.0110
Cl1	4c	0.1036	0.2500	0.3192	1.000	0.0184
O1	4c	0.3623	0.2500	0.7220	1.000	0.0145
O2	8d	0.2747	0.1832	0.8719	1.000	0.0059
O3	8d	0.6746	0.4350	0.9457	1.000	0.0323
O4	8d	0.2616	0.5006	0.8389	1.000	0.0117
O5	8d	0.9741	0.1019	0.0770	1.000	0.0400
B1	8d	0.7853	0.4433	0.0935	1.000	0.0120
B2	4c	0.2969	0.2500	0.8869	1.000	0.0140

Table S3 Bond distance (Å) of BSBOC:0.025Eu^{2+}

Sr1/Eu1-O2	2.81865(10)	Sr2/Eu2-O4	2.61251(7)
Sr1/Eu1-O3	2.61406(11)	Sr2/Eu2-O4	2.56248(8)
Sr1/Eu1-O3	2.71517(9)	Sr2/Eu2-O5	2.82811(14)
Sr1/Eu1-O4	2.75112(9)	(average)	2.6202988
Sr1/Eu1-O4	3.07060(11)	Sr3/Eu3-O2(×2)	2.79106(8)
Sr1/Eu1-O4	3.03378(11)	Sr3/Eu3-O1	2.53240(11)
Sr1/Eu1-O5	2.71484(12)	Sr3/Eu3-O5(×2)	2.47674(11)
Sr1/Eu1-O5	3.07652(14)	Sr3/Eu3-Cl1	2.95260(11)
Sr1/Eu1-Cl1	3.19762(11)	Sr3/Eu3-Cl1	2.88921(13)
(average)	2.8880429	(average)	2.7014045
Sr2/Eu2-O1	2.60056(11)		
Sr2/Eu2-O2	2.49905(7)		
Sr2/Eu2-O2	2.49966(8)		
Sr2/Eu2-O3	2.56037(9)		
Sr2/Eu2-O3	2.79960(9)		

Table S4 Quantum efficiencies of BSBOC:0.025Eu^{2+} and commercial YAG:Ce^{3+}

	BSBOC:0.025Eu^{2+} (%)	YAG:Ce^{3+} (%)
Internal QE	55.5	94.8
Absorption	45.0	85.2
External QE	25.0	80.7

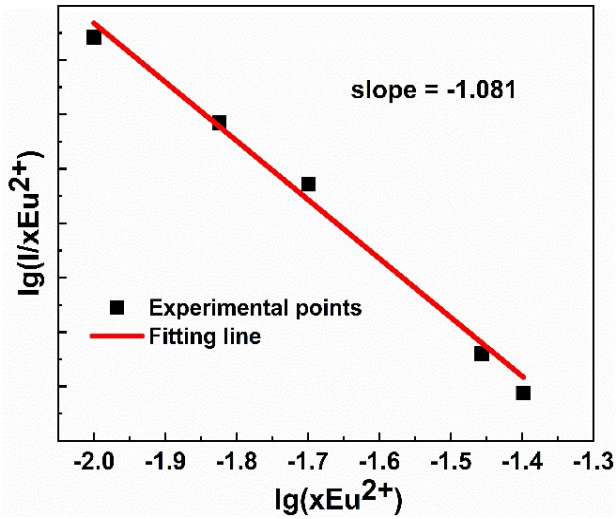

Fig. S1 Relationship of lg(I/xEu^{2+}) with lg(xEu^{2+}) in BSBOC:xEu^{2+} phosphors under 450 nm excitation.

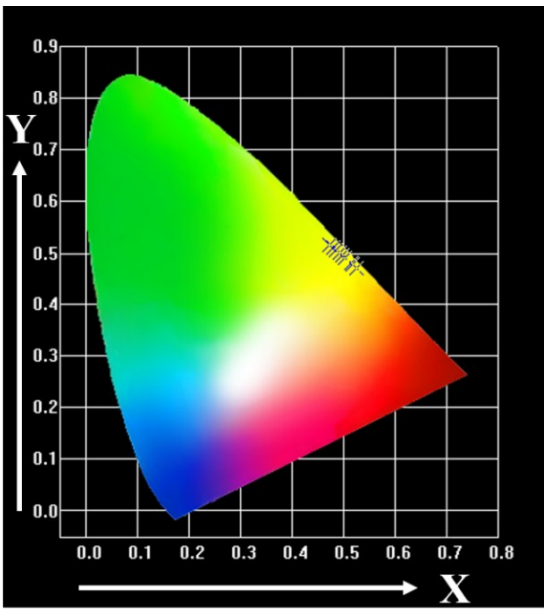

Fig. S2 CIE coordinates of BSBOC:0.025Eu^{2+} at different temperature (T = 273–473K).

Table S5 CIE coordinates of BSBOC:0.025Eu^{2+} at different temperature (T = 273–473 K).

Temperature (K)	CIE coordinates (x, y)
273	(0.524, 0.471)
298	(0.518, 0.477)
323	(0.514, 0.480)
348	(0.503, 0.490)
373	(0.497, 0.495)
398	(0.492, 0.499)
423	(0.484, 0.506)
448	(0.480, 0.509)
473	(0.472, 0.515)

Reference

1. J. P. Perdew and K. Burke, *Phys. Rev. B*, 1996, **77**, 3865-3868.

2. G. Kresse and J. Furthmüller, *Comp. Mater. Sci*., 1996, **6**, 15-50.

3. G. Kresse and J. Hafner, *Phys. Rev. B*, 1993, **47**, 558-561.

4. G. Kresse and J. Hafner, *Phys. Rev. B*, 1994, **49**, 14251-14269.

5. G. Kresse and J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169-11186.

6. H. J. Monkhorst and J. D. Pack, *Phys. Rev. B*, 1976, **13**, 5188-5192.

7. K. O. Obodo, C. N. M. Ouma, G. Gebreyesus, J. T. Obodo, S. O. Ezeonu and B. Bouhafs, *Mater. Res. Express*, 2019, **6**, 106307.