

Supporting Information

Achieving the white emission by site-selective occupation of Eu^{2+} in $\text{K}_2\text{BaSr}(\text{PO}_4)_{2-x}(\text{BO}_3)_x:\text{Eu}^{2+}$

Guo-Dong Xie^a, Jia-Yong Si^{*a}, Gui-Hua Li^b, Ge-Mei Cai^{*b}, Zhi-Peng Wang^c and
Xiao-Jun Wang^{*d}

^aCollege of Mechanical and Electrical Engineering, Central South University of
Forestry and Technology, Changsha, Hunan 410004, China

^bSchool of Materials Science and Engineering, Central South University, Changsha,
Hunan 410083, China

^cState Key Laboratory of Advanced Design and Manufacturing for Vehicle Body,
Hunan University, Changsha, Hunan 410082, China

^dDepartment of Physics, Georgia Southern University, Statesboro, Georgia 30460,
United States

*Correspondence: sjy98106@163.com (J.-Y. Si) or caigemei@csu.edu.cn (G.-M. Cai) or
xwang@georgiasouthern.edu (X.-J. Wang).

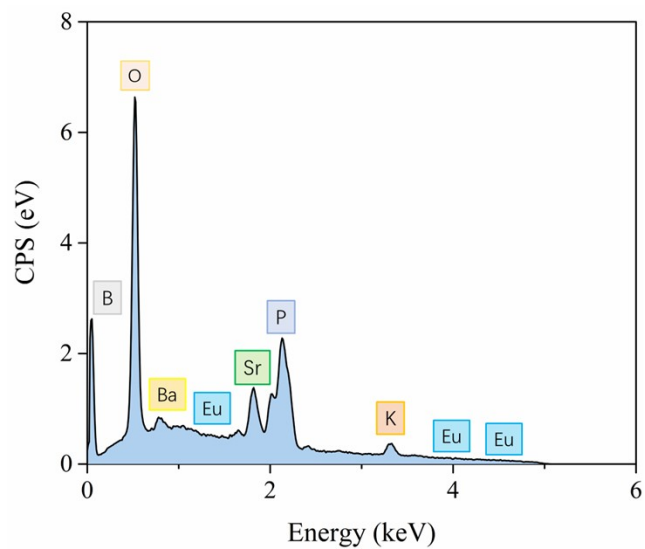


Figure S1. The elemental mapping spectrum of $\text{KBaSP}_{1.8}\text{B}_{0.2}:\text{0.04Eu}^{2+}$.

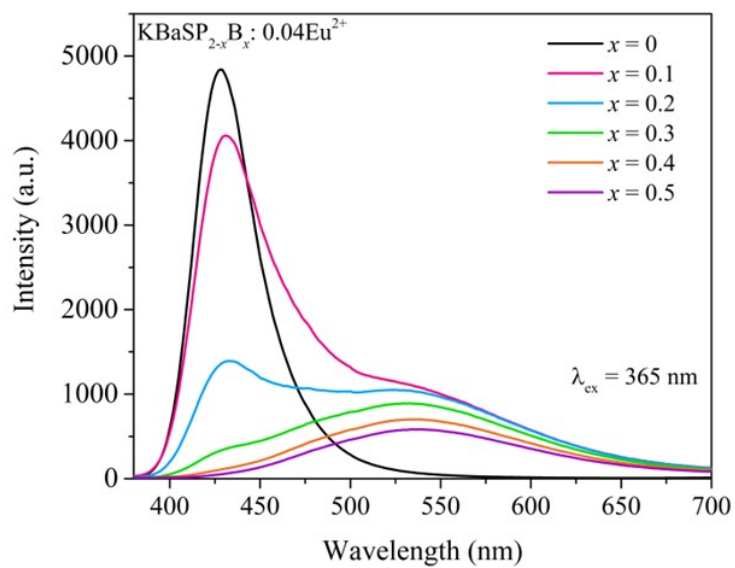


Figure S2. The photoluminescence spectra of $\text{KBaSP}_{2-x}\text{B}_x:\text{0.04Eu}^{2+}$ ($x = 0, 0.1, 0.2, 0.3, 0.4, 0.5$) samples.

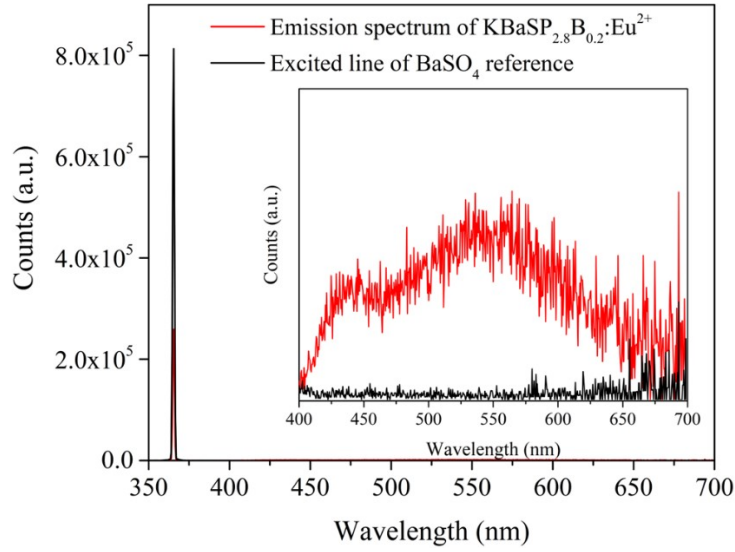


Figure S3. Excitation line of BaSO₄ and the emission spectra of KBaSP_{1.8}B_{0.2}:0.04Eu²⁺ sample collected by using an integrating sphere. The inset shows the magnification of the BaSO₄ and $x = 0.2$ emission spectra.

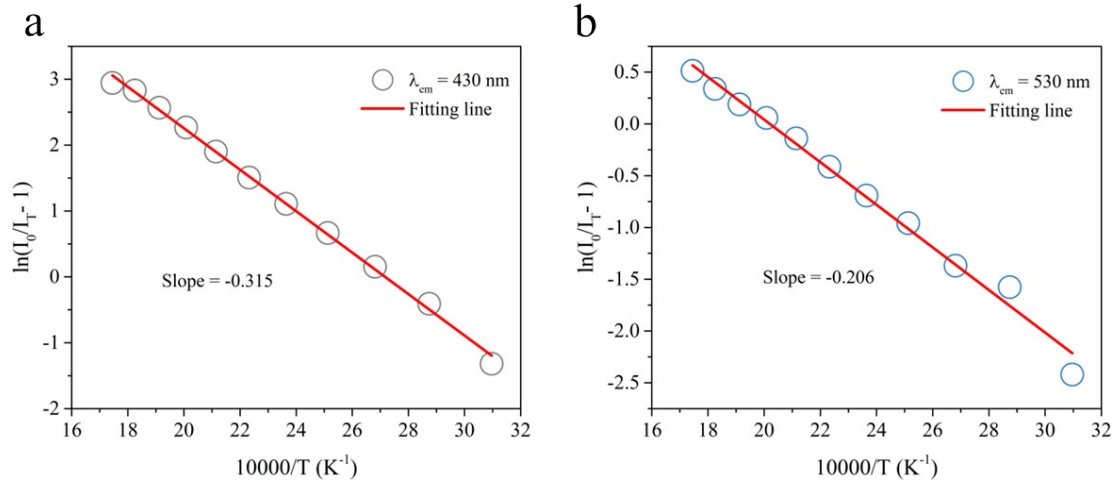


Figure S4. The plot of $\ln(I_0/I_T - 1)$ versus $10^4/T$ at two emission band centered at 430 nm and 530 nm, respectively.

Table S1. Lattice parameters obtained from XRD Rietveld refinements of $\text{KBaSP}_{1.8}\text{B}_{0.2}:0.04\text{Eu}^{2+}$.

Compound	$\text{KBaSP}_{1.8}\text{B}_{0.2}:0.04\text{Eu}^{2+}$
space group	$P n m a$
a (Å)	7.702(5)
b (Å)	10.002(9)
c (Å)	5.6422(2)
V (Å ³)	434.5(3)
R_{wp} (%)	8.372
R_p (%)	6.011

Table S2 The refined atomic positions of $\text{KBaSP}_{1.8}\text{B}_{0.2}:0.04\text{Eu}^{2+}$ obtained from the Rietveld analysis.

Atom	Site	X	Y	Z	B_{iso} (Å ²)	Occ.
Ba1	4c	-0.00474	0.25000	0.19835	0.06773	0.24750
Sr1	4c	-0.00474	0.25000	0.19835	0.06773	0.24750
P1	4c	0.23162	0.25000	0.90553	0.0000	0.45000
K1	4c	0.16367	0.25000	0.58470	0.0000	0.48000
O1	8d	0.19955	-0.04708	0.33765	0.10273	1.00000
O2	4c	0.02705	0.25000	0.90451	1.34007	0.50000
O3	4c	0.30910	0.25000	0.05182	0.0000	0.50000
Eu1	4c	-0.00474	0.25000	0.19835	0.06773	0.00500
Eu2	4c	0.16367	0.25000	0.58470	0.0000	0.02000
B1	4c	0.23162	0.25000	0.90553	0.0000	0.05000

Table S3. The chromaticity coordinates of $\text{KBaSP}_{2-x}\text{B}_x:0.04\text{Eu}^{2+}$ ($x = 0, 0.1, 0.2, 0.3, 0.4, 0.5$) samples excited at 365 nm.

Compounds	C_x	C_y	CCT(K)
$\text{KBaSP}: \text{Eu}^{2+}$	0.1598	0.0376	/
$\text{KBaSP}_{1.9}\text{B}_{0.1}: \text{Eu}^{2+}$	0.2164	0.1958	/
$\text{KBaSP}_{1.8}\text{B}_{0.2}: \text{Eu}^{2+}$	0.2620	0.3066	10857
$\text{KBaSP}_{1.7}\text{B}_{0.3}: \text{Eu}^{2+}$	0.3071	0.4089	6381
$\text{KBaSP}_{1.6}\text{B}_{0.4}: \text{Eu}^{2+}$	0.3312	0.4531	5594
$\text{KBaSP}_{1.5}\text{B}_{0.5}: \text{Eu}^{2+}$	0.3423	0.4708	5329

The correlated color temperature (CCT) is an important index to evaluate the phosphor performance, and its value can be calculated by McCamy's theoretical formula:

$$CCT = -449n^3 + 3525n^2 - 6823.3n + 5520.33 \quad (1)$$

where $n = (x - x_e)/(y - y_e)$ is the reciprocal of the slope, and x_e and y_e are constants equal to 0.332 and 0.186, respectively.