Supporting Information:

An efficient blue phosphor with high thermal stability for lighting and optical pressure sensor applications

Hang Chen,[†] Takatoshi Seto,[†,*] Yuhua Wang[†,*]

[†] *National and Local Joint Engineering Laboratory for Optical Conversion Materials and Technology of National Development and Reform Commission, School of Materials and Energy Lanzhou University Lanzhou, 730000, China*

* *Corresponding author, email:* seto@lzu.edu.cn *and* wyh@lzu.edu.cn

1. Procedure of LED-device fabrication

The raw materials include Epoxy resin AB glue, 395 nm LED chip, red and green phosphor ($CaAlSiN_3$: Eu^{2+} and $(BaSr)_2SiO_4$: Eu^{2+}) and as-prepared sample NCMPO:0.03Eu^{2+}.

Firstly, we mixed the phosphors and ground thoroughly, the mass ratio of red, green and blue phosphor is about 1:1:1.2, and the total mass is 0.015g. There are slightly more blue phosphors due to the reabsorption of red and green phosphors in the blue region.

Secondly, about 0.02 g main agent A glue was weighted, and mix the weighted A glue and phosphor and stir evenly, then add 0.08g curing agent B glue, and stir for five minutes after adding B glue.

Finally, the defoamed mixture is dripped onto a 395 nm LED chip, and put the chip into the oven at 60 °C for 40 minutes and then at 135 °C for 90 minutes. After that, the white LED device was successfully fabricated.

Table S1 The atomic coordinates of $Na_3CsMg_7(PO_4)_6$ obtained from the Rietveld Refinement

Atom	Position	x/a	y/b	z/c
Na1	8f	0.5521(6)	0.2519(2)	0.0216(6)
Na2	8f	0.2834(2)	0.238(4)	0.0399(1)
Cs1	4e	0	0.2532(4)	1/4
Mg1	4e	1/2	0.1117(1)	1/4
Mg2	8f	0.1790(7)	0.4850(9)	0.1377(6)

Mg3	8f	0.2511(2)	-0.258(4)	0.0336(1)
Mg4	4e	1/2	0.3998(1)	1/4
Mg5	8f	0.3154(7)	0.5260(7)	0.3672(5)
P1	8f	0.2932(4)	0.2603(1)	0.2806(4)
P2	8f	0.4183(7)	0.0077(7)	0.0806(5)
P3	8f	0.4025(6)	0.4949(6)	0.0793(4)
O1	8f	0.5455(1)	0.0158(2)	0.1535(9)
O2	8f	0.3237(1)	0.4563(2)	0.1432(9)
O3	8f	0.5370(1)	0.5099(1)	0.1411(8)
O4	8f	0.4154(9)	0.2402(2)	0.2902(8)
O5	8f	0.3531(8)	0.0589(1)	0.1316(7)
O6	8f	0.3802(9)	0.3977(9)	0.0099(7)
O7	8f	0.4032(1)	0.0624(1)	-0.106(8)
O8	8f	0.3912(1)	-0.1212(1)	0.05401(8)
O9	8f	0.3853(1)	0.6094(1)	0.0189(1)
O10	8f	0.2542(9)	0.4154(1)	0.2783(8)
O11	8f	0.2885(1)	0.1648(1)	0.3583(8)
O12	8f	0.2063(1)	0.2028(2)	0.1769(8)

Table S2 The bond lengths (Å) of $Na_3CsMg_7(PO_4)_6$ obtained from the Rietveld Refinement

Type of bond	Bond length	Type of bond	bond length
Cs(1)-O(8)	3.1130	Mg(2)-O(10)	2.1454
Cs(1)-O(8)	3.1130	Mg(2)-O(11)	1.9644
Cs(1)-O(3)	3.2381	Mg(3)-O(9)	2.2590
Cs(1)-O(3)	3.2381	Mg(3)-O(9)	2.3001
Cs(1)-O(12)	3.2876	Mg(3)-O(8)	2.2085
Cs(1)-O(12)	3.2876	Mg(3)-O(8)	1.2325
Cs(1)-O(1)	3.3406	Mg(3)-O(11)	2.1013
Cs(1)-O(1)	3.3406	Mg(3)-O(11)	3.1053
		Mg(4)-O(4)	2.2346
Na(1)-O(6)	2.3400	Mg(4)-O(4)	2.2346
Na(1)-O(8)	2.3593	Mg(4)-O(2)	2.2898
Na(1)-O(7)	2.4625	Mg(4)-O(2)	2.2898
Na(1)-O(9)	2.1375	Mg(4)-O(3)	2.2566
Na(1)-O(11)	2.5778	Mg(4)-O(3)	2.2566
Na(1)-O(4)	2.7146	Mg(5)-O(12)	1.9946
Na(2)-O(6)	2.2598	Mg(5)-O(10)	1.7529
Na(2)-O(6)	2.4055	Mg(5)-O(6)	2.1971
Na(2)-O(7)	2.7219	Mg(5)-O(5)	2.1812
Na(2)-O(5)	2.3456	Mg(5)-O(3)	1.9408

Na(2)-O(7)	3.0936	Mg(5)-O(9)	2.6078
Na(2)-O(2)	2.7662		
Na(2)-O(12)	2.6949	P(1)-O(12)	1.6740
Na(2)-O(5)	3.3493	P(1)-O(10)	1.7292
		P(1)-O(11)	1.6001
Mg(1)-O(4)	1.9917	P(1)-O(4)	1.5191
Mg(1)-O(4)	1.9917	P(2)-O(8)	1.4428
Mg(1)-O(1)	2.0767	P(2)-O(7)	1.4737
Mg(1)-O(1)	2.0767	P(2)-O(5)	1.4595
Mg(1)-O(5)	2.1233	P(2)-O(1)	1.5742
Mg(1)-O(5)	2.1233	P(3)-O(9)	1.5063
Mg(2)-O(7)	1.9058	P(3)-O(6)	1.4439
Mg(2)-O(1)	1.8395	P(3)-O(3)	1.6106
Mg(2)-O(2)	1.8364	P(3)-O(2)	1.7145

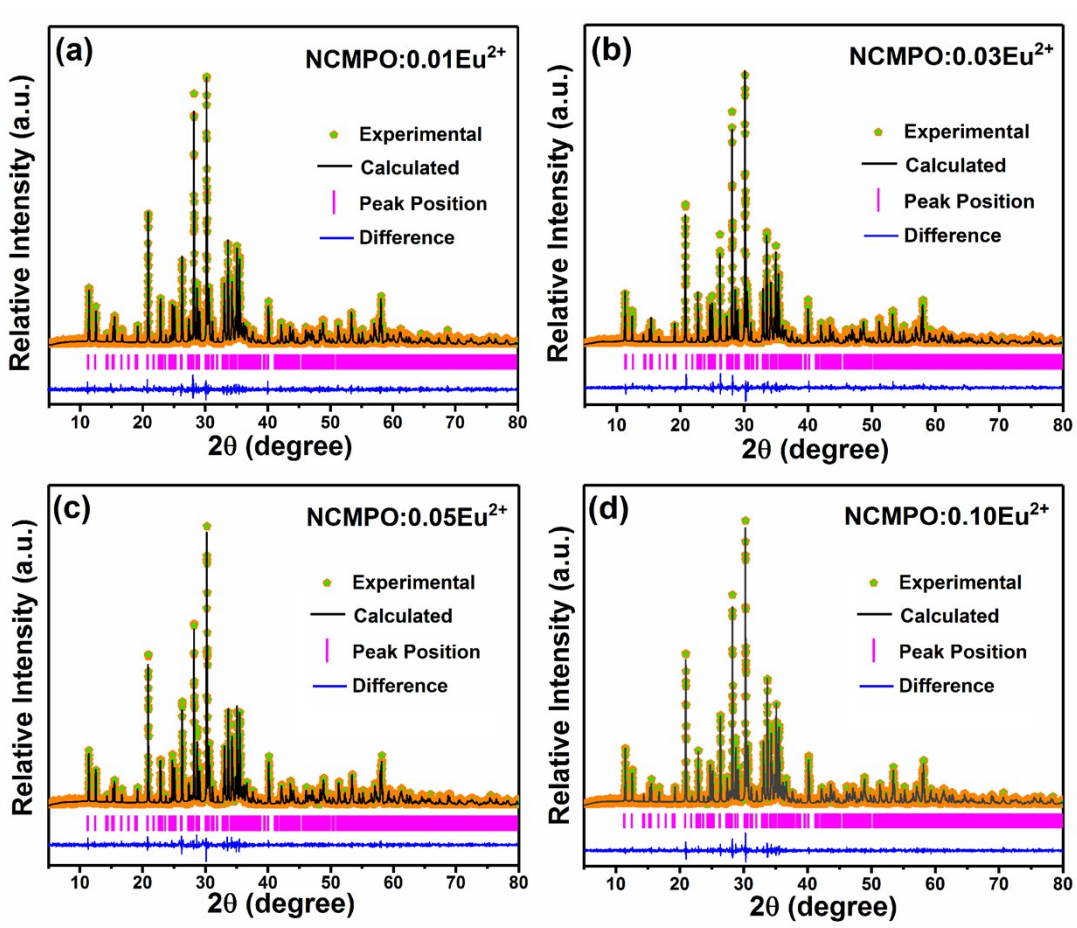

Figure. S1 the Rietveld refinement XRD pattern of NCMPO: xEu^{2+} (x=0.01, 0.03, 0.05, 0.10)

Table S3 The crystallographic data of NCMPO:0.01Eu^{2+} by Rietveld refinement	
Formula	$Na_3Cs_{0.99}Eu_{0.01}Mg_{6.99}Li_{0.01}(PO_4)_6$
Crystal system	monoclinic
Space group	C 1 2/c 1 (15)
Cell parameters (Å)	a=12.7322(2) b= 10.7006(1) c= 15.5281(2)
Cell ratio	b/c=0.6891 c/a=1.2196 a/b=1.1899
Cell volume	1947.13(4) $Å^3$
Calculated density	3.37397 g/cm^3
Z	4
Reliability factors	R_{wp}=9.64% R_p=7.59% χ^2= 1.203

Table S4 The crystallographic data of NCMPO: 0.03$Eu^{2+}$by Rietveld refinement	
Formula	$Na_3Cs_{0.97}Eu_{0.03}Mg_{6.97}Li_{0.03}(PO_4)_6$
Crystal system	monoclinic
Space group	C 1 2/c 1 (15)
Cell parameters (Å)	a=12.7263(2) b= 10.6969(1) c= 15.5196(2)
Cell ratio	b/c=0.6893 c/a=1.2195 a/b=1.1897
Cell volume	1945.43(4) $Å^3$
Calculated density	3.37893 g/cm^3
Z	4
Reliability factors	R_{wp}=10.09% R_p=7.58% χ^2= 1.164

Table S5 The crystallographic data of NCMPO: 0.05Eu^{2+} by Rietveld refinement	
Formula	$Na_3Cs_{0.95}Eu_{0.05}Mg_{6.95}Li_{0.05}(PO_4)_6$
Crystal system	monoclinic
Space group	C 1 2/c 1 (15)
Cell parameters (Å)	a=12.7252(2) b= 10.6967 (1) c= 15.5193(2)
Cell ratio	b/c=0.6893 c/a=1.2196 a/b=1.1896
Cell volume	1943.67(4) $Å^3$
Calculated density	3.38022 g/cm^3
Z	4
Reliability factors	R_{wp}=10.19% R_p=8.03% χ^2= 1.267

Table S6 The crystallographic data of NCMPO: 0.10Eu^{2+} by Rietveld refinement	
Formula	$Na_3Cs_{0.90}Eu_{0.10}Mg_{6.90}Li_{0.10}(PO_4)_6$
Crystal system	monoclinic
Space group	C 1 2/c 1 (15)
Cell parameters (Å)	a=12.7233(2) b= 10.6900 (1) c= 15.5151(2)
Cell ratio	b/c=0.6890 c/a=1.2194 a/b=1.1902
Cell volume	1942.53(4) $Å^3$
Calculated density	3.38062 g/cm^3
Z	4
Reliability factors	R_{wp}=9.97% R_p=8.13% χ^2= 1.294

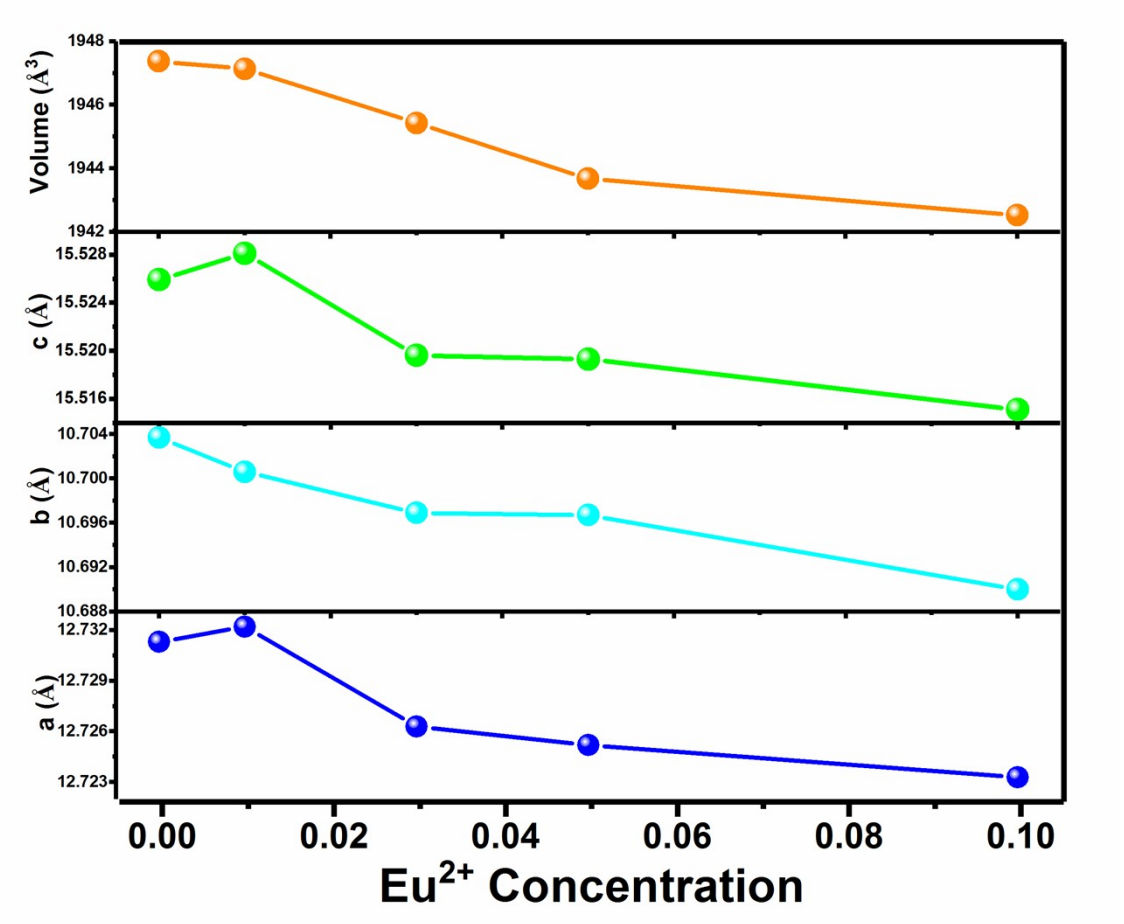

Figure. S2 The change of the cell parameters with different Eu^{2+} concentration

Table. S7 The data on EDX of the samples

Atom / Samples	Na	Cs	Mg	P	Eu
0	3.09	1.00	6.91	6	0
0.01	3.02	0.99	6.98	6	0.01
0.02	2.99	0.98	6.96	6	0.02
0.03	3.01	0.97	6.95	6	0.03
0.04	3.00	0.96	6.95	6	0.04
0.05	3.01	0.95	6.94	6	0.05
0.07	2.97	0.93	6.93	6	0.07
0.10	3.01	0.90	6.90	6	0.10

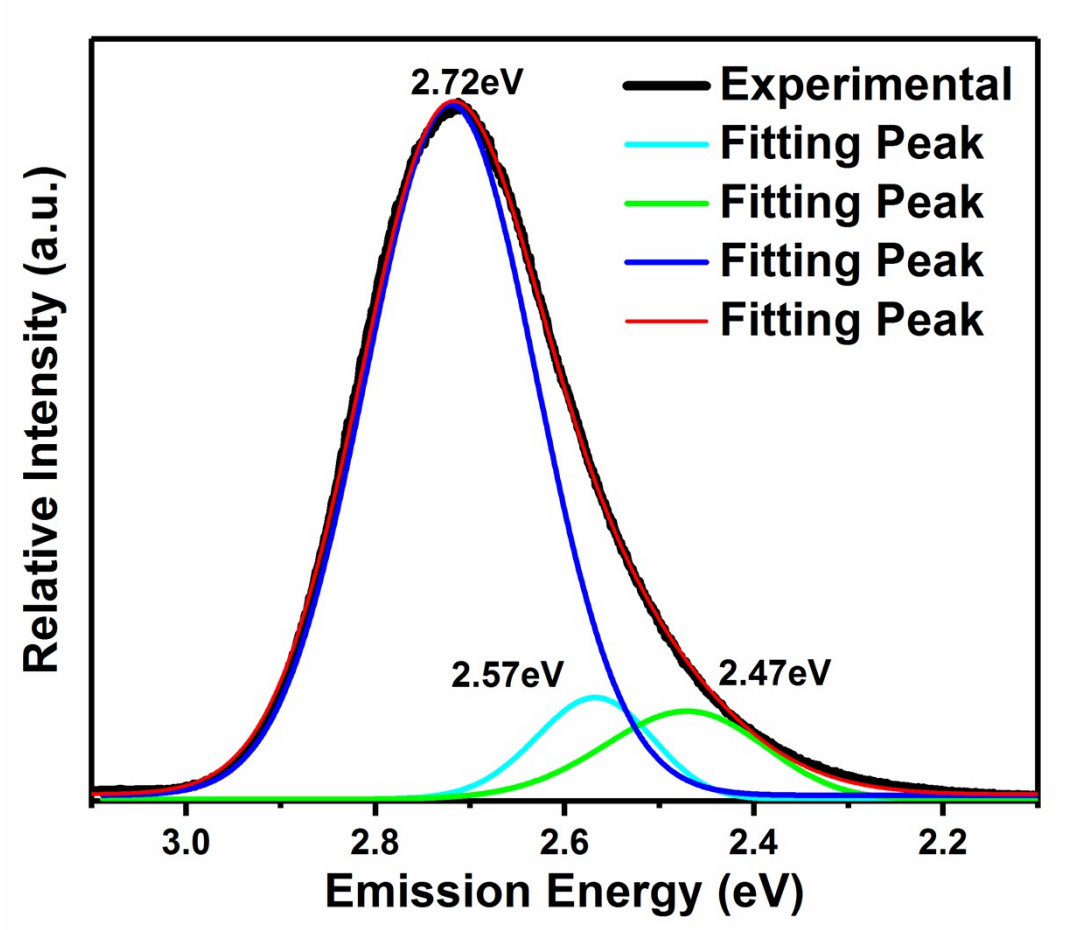

Figure. S3 The emission spectrum with Guassian fitting

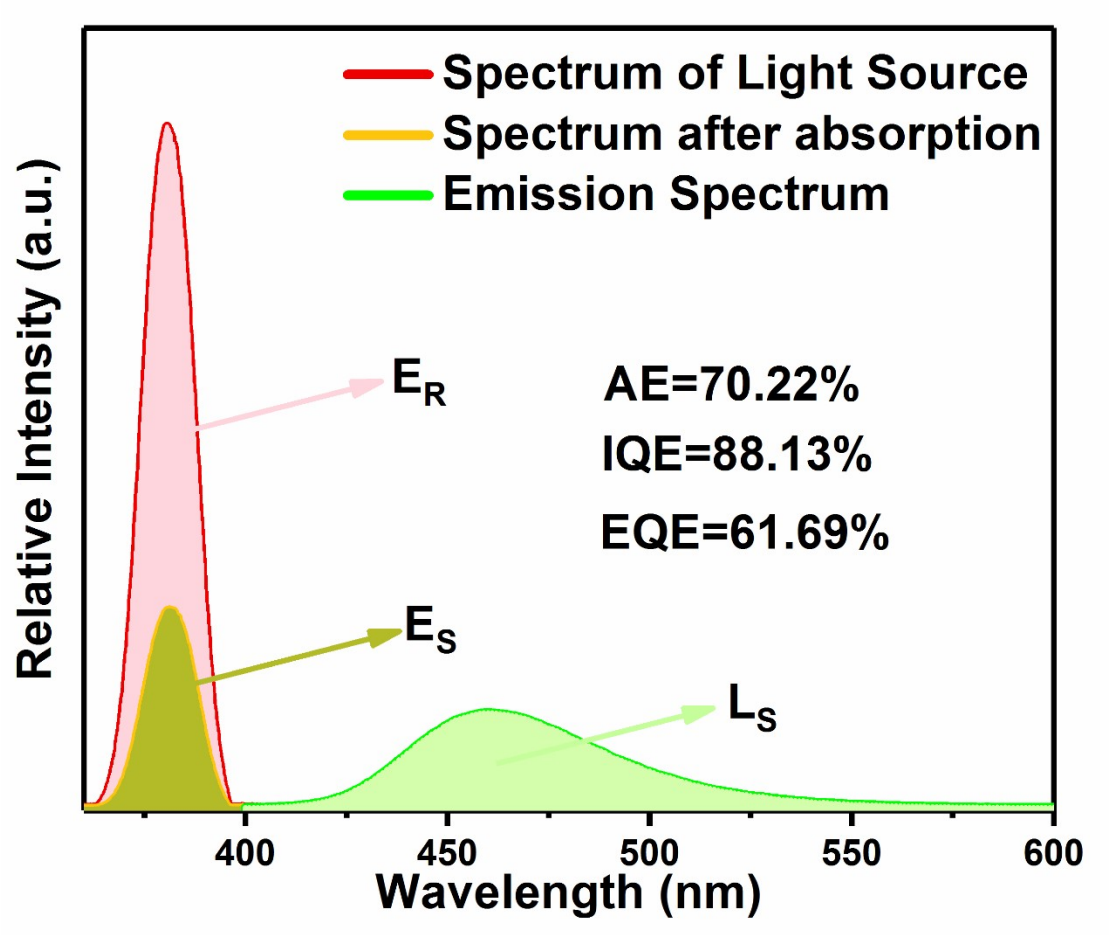

Figure. S4 The spectra of light sorce and NCMPO: $0.03Eu^{2+}$ collected by using an integrating sphere

The absorption efficiency (AE), internal quantum efficiency (IQE) and external quantum efficiency (EQE) can be calculated by using the following equations:

$$AE = \frac{\int E_R - \int E_S}{\int E_R}$$

$$IQE = \frac{\int L_S}{\int E_R - \int E_S}$$

$$EQE = AE \times IQE = \frac{\int L_S}{\int E_R}$$

in which E_S stands for the spectrum of light used for exciting the phosphor, L_S

represents the emission spectrum of the phosphor, and E_R is the spectrum of excitation light without phosphor in sphere.)