Electronic Supplementary Material (ESI) for RSC Advances.
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Electronic supplementary material

Red phosphor based on Eu^{3+}- isoelectronically doped Ba_2SiO_4 obtained via sol-gel route for solid state lightning.

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Experimental procedure

Table ES1. Doping proportions and amount of reagents added, assuming 2.0000 g of the product. The Eu^{3+} concentration was isoelectronically varied from 1 to 5 %, i.e., keeping equivalent positive and negative charges according to the sum of cation charges and SiO_4^{4-} charges ($3n_{Eu^{3+}} + 2n_{Ba^{2+}} = +4$, where $n_{Ba^{2+}}$ and $n_{Eu^{3+}}$ are the mol amount of Ba^{2+} and Eu^{3+}, respectively).

	Eu^{3+} doping		**Structural formula**	**Molecular weight / g/mol**	**Ba^{2+} acetate mass (g)**	**Volume (mL)**	
% [a]	**at %[b]**	**ch%[c]**				**Eu^{3+} acetate***	**TEOS****
5 %	5.13 at%	7.5 ch%	$Ba_{1.85}Eu_{0.1}SiO_4$	361.4125	2.6149	11.07	10.06
4%	4.08 at%	6 ch%	$Ba_{1.88}Eu_{0.08}SiO_4$	362.4944	2.6494	8.83	10.03
3 %	3.05 at%	4.5 ch%	$Ba_{1.91}Eu_{0.06}SiO_4$	363.5763	2.6836	4.66	10.00
2 %	2.02 at%	3 ch%	$Ba_{1.94}Eu_{0.04}SiO_4$	364.6582	2.7175	4.39	9.97
1 %	1.00 at%	1.5 ch%	$Ba_{1.97}Eu_{0.02}SiO_4$	365.7401	2.7517	2.19	9.94
Undoped	-	-	Ba_2SiO_4	366.8220	2.7852	-	9.91

[a] Eu^{3+}-doping percentage in relation to 2 mols of Ba^{2+} in the undoped Ba_2SiO_4. [b] Eu^{3+}-doping percentage in relation to the total cation mol amount for each sample; [c] Eu^{3+}-doping percentage in relation to the total cation charge in each sample.

*0.05 mol.L^{-1}in acetic acid solution

**0.55 mol.L^{-1}in isopropyl alcohol solution.

Table ES2

Table ES2. The full width at half maximum, position, band area and height for the (ν_1) ν_s and (ν_3) ν_{as} vibrational mode in the Raman spectra for the undoped and doped-phosphors.

Band	Area / arb. units	Position/cm^{-1}	FWHM/cm^{-1}	Height/arb. units
5 %				
(ν_1) ν_s (SiO_4)	117411	822	7	10471
	44141	856	12	2331
(ν_3) ν_{as} (SiO_4)	12893	885	10	749
	25576	909	10	1530
4 %				
(ν_1) ν_s (SiO_4)	180867	822	7	15440
	59486	857	11	3236
(ν_3) ν_{as} (SiO_4)	29749	885	16	1158
	41930	909	11	2314
3 %				
(ν_1) ν_s (SiO_4)	113725	822	8	8207
	40250	857	13	1945
(ν_3) ν_{as} (SiO_4)	18011	885	14	766
	38062	909	16	1439
2 %				
(ν_1) ν_s (SiO_4)	172552	822	8	12325
	59749	857	13	2957
(ν_3) ν_{as} (SiO_4)	36740	885	17	1310
	55204	909	16	2156
1 %				
(ν_1) ν_s (SiO_4)	298999	822	7	25199
	95598	857	11	5250
(ν_3) ν_{as} (SiO_4)	50187	885	16	1928
	76444	909	12	3796
Undoped				
(ν_1) ν_s (SiO_4)	215292	822	6	20913
	65351	857	10	4093
(ν_3) ν_{as} (SiO_4)	26499	885	11	1533
	46811	909	10	3036

Crystallite size determination by Scherrer method.

The crystallite size was determinate according to Equation ES1.[1]

$$\beta_p = \frac{c\lambda}{\varepsilon cos\theta} \text{(Equation ES1)}$$

Where β_p is the full width at half maximumin radians of a given $h\ k\ l$ reflection peak, ε, in the corresponding direction to the ($h\ k\ l$) and c is a constant that depends on the reflection symmetry which usually is given as 0.9 for non-spherical crystallite. To calculate the samples crystallite size the three most intense peaks observed in the diffraction pattern related to the (1 2 1), (2 1 1) and (0 3 1) plans were considered.

Figure ES1

Figure ES1. Scanning electron microscopy images of undoped and Eu^{3+}-doped Ba_2SiO_4 prepared by the sol-gel method.

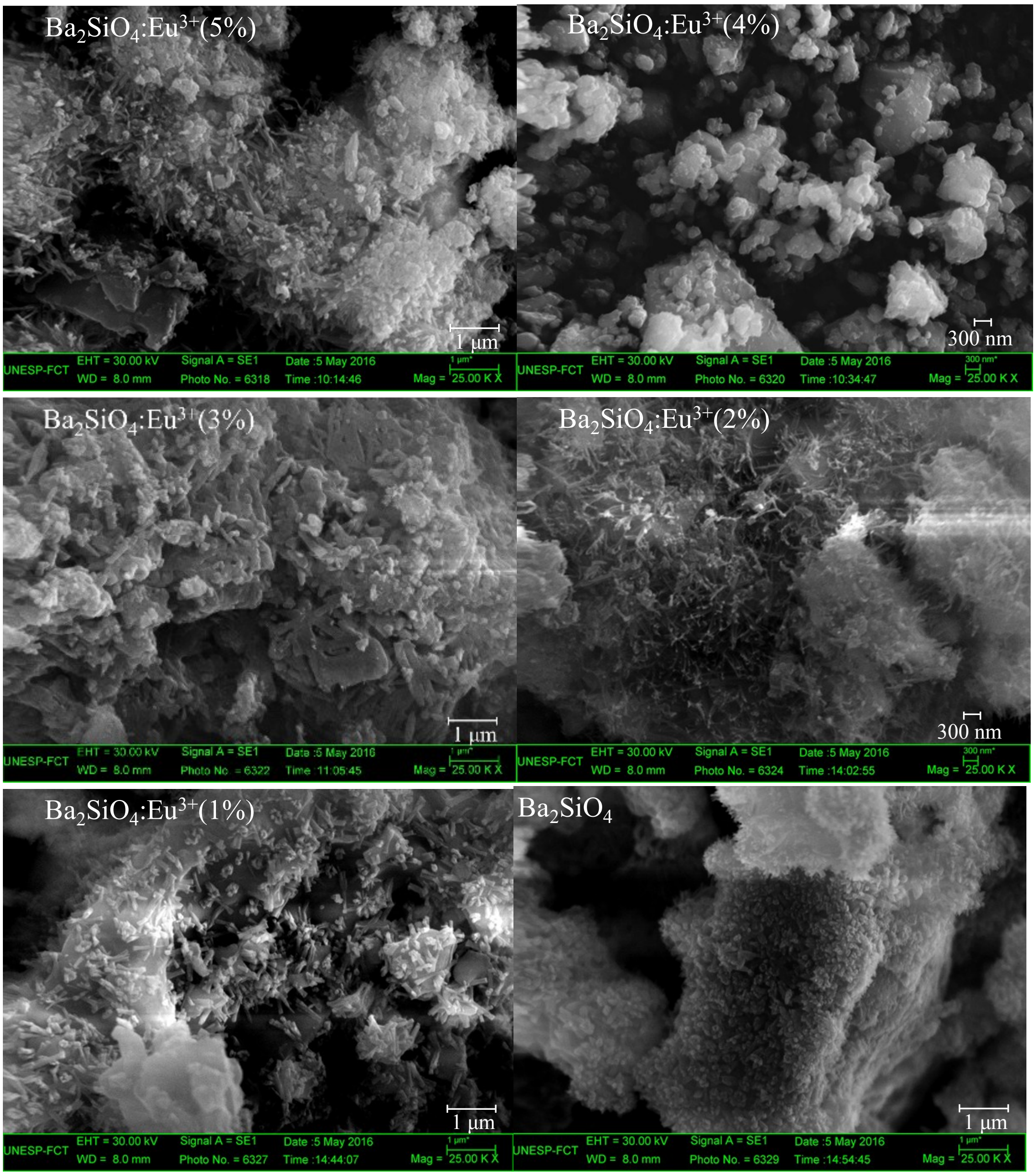
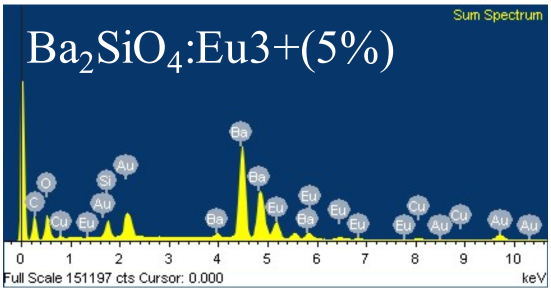


Figure ES2

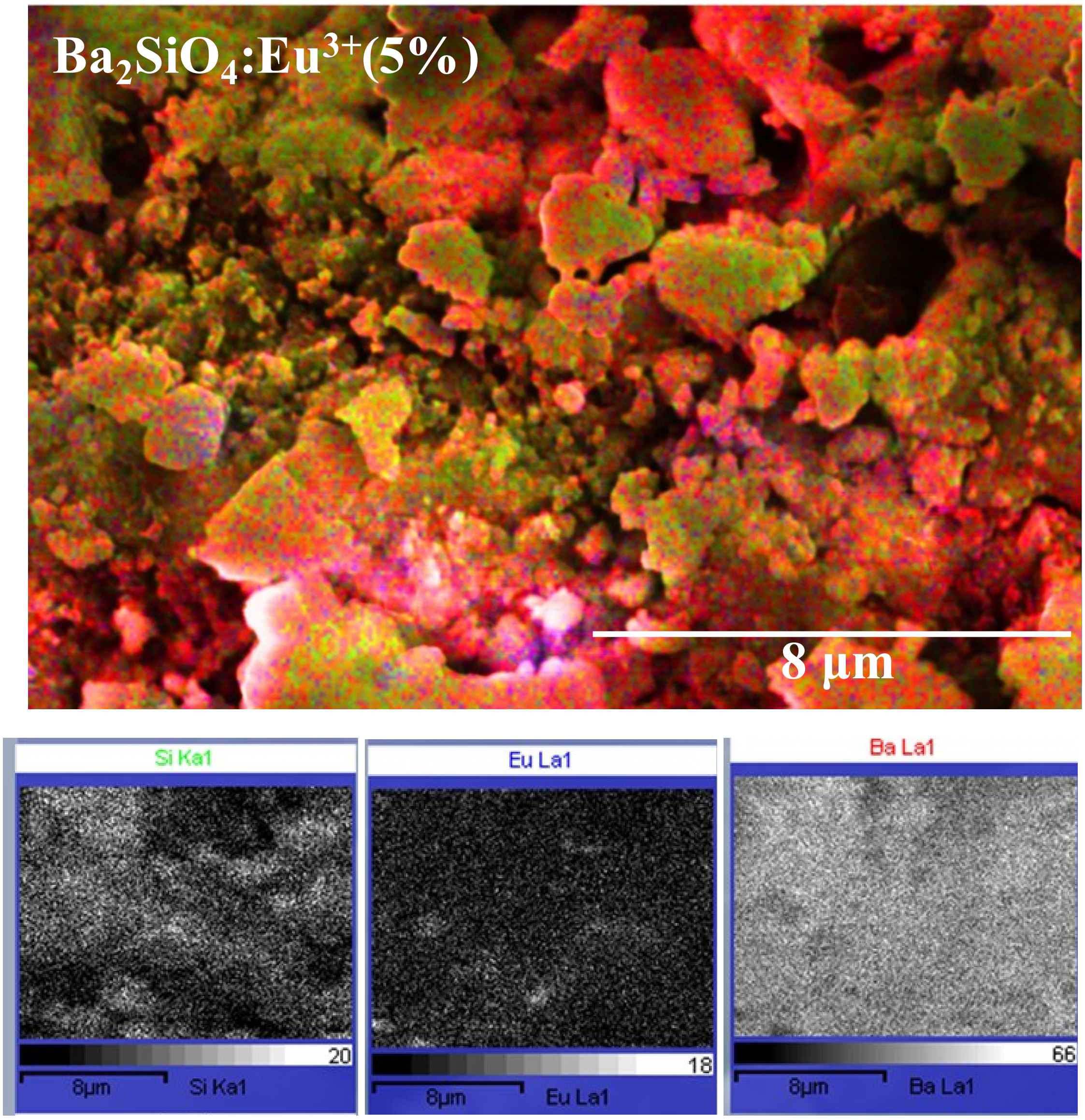
Figure ES2. (a) Energy Dispersive Spectroscopy (EDS) for Eu^{3+}-doped Ba_2SiO_4[a] and (b) chemical mapping by EDS.



[a] The phosphor was analyzed by energy dispersive spectroscopy (X OXFORD *Instruments* model INCAx-act) to identify elements on the particle surfaces. The elements Ba, Eu, Si and O observed are from the $Ba_2SiO_4:Eu^{3+}$ phase, the element Au was used to metalize the sample and the element C attributed to the formation of amorphous carbonate on the particles surface, as it is discussed in the FTIR results.

Figure ES3

Figure ES3. Chemical mapping by EDS for $Ba_2SiO_4:Eu^{3+}$(5%)[a].



[a] Chemical mapping obtained by EDS showing the homogeneous distribution of the elements Ba, Eu and Si in an agglomerate of particles. The element Ba is shown in red, Si in green and Eu in blue. Also, the homogeneous distribution can be seen at the bottom of the figure.

Figure ES4

Figure ES4. Bandgap calculation for undoped and Eu^{3+}-doped Ba_2SiO_4 prepared by sol-gel method.

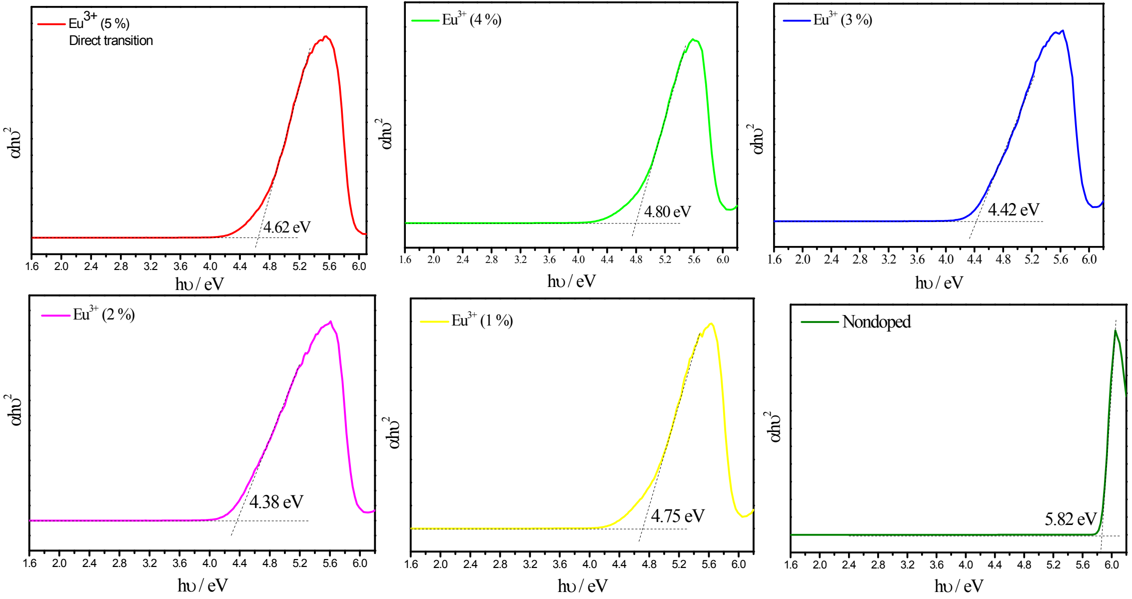


Figure ES5

Figure ES5. Kubelka-Munk approximation for Ba_2SiO_4:Eu^{3+}(5%) considering direct and indirect transition.

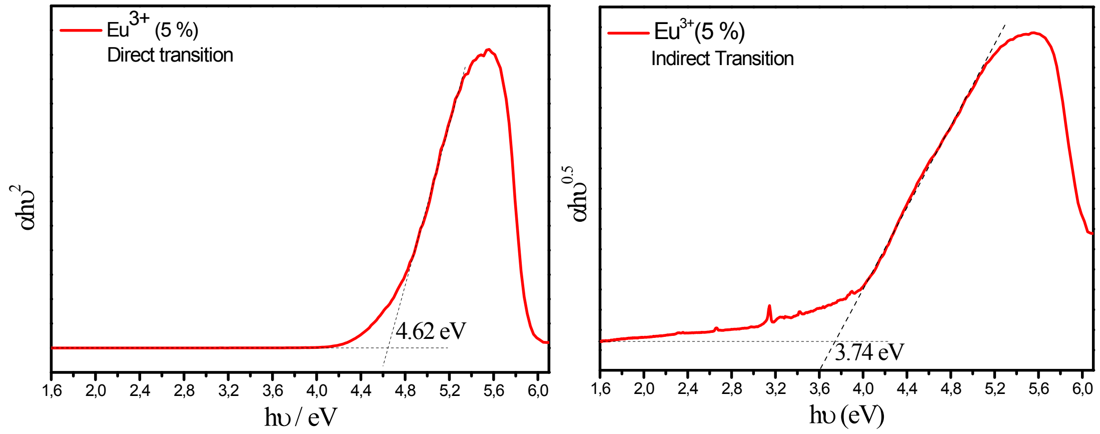


Figure ES6

Figure ES6. Emission spectra of $Ba_2SiO_4:Eu^{3+}$ powder samples under 250 nm measured at room temperature.

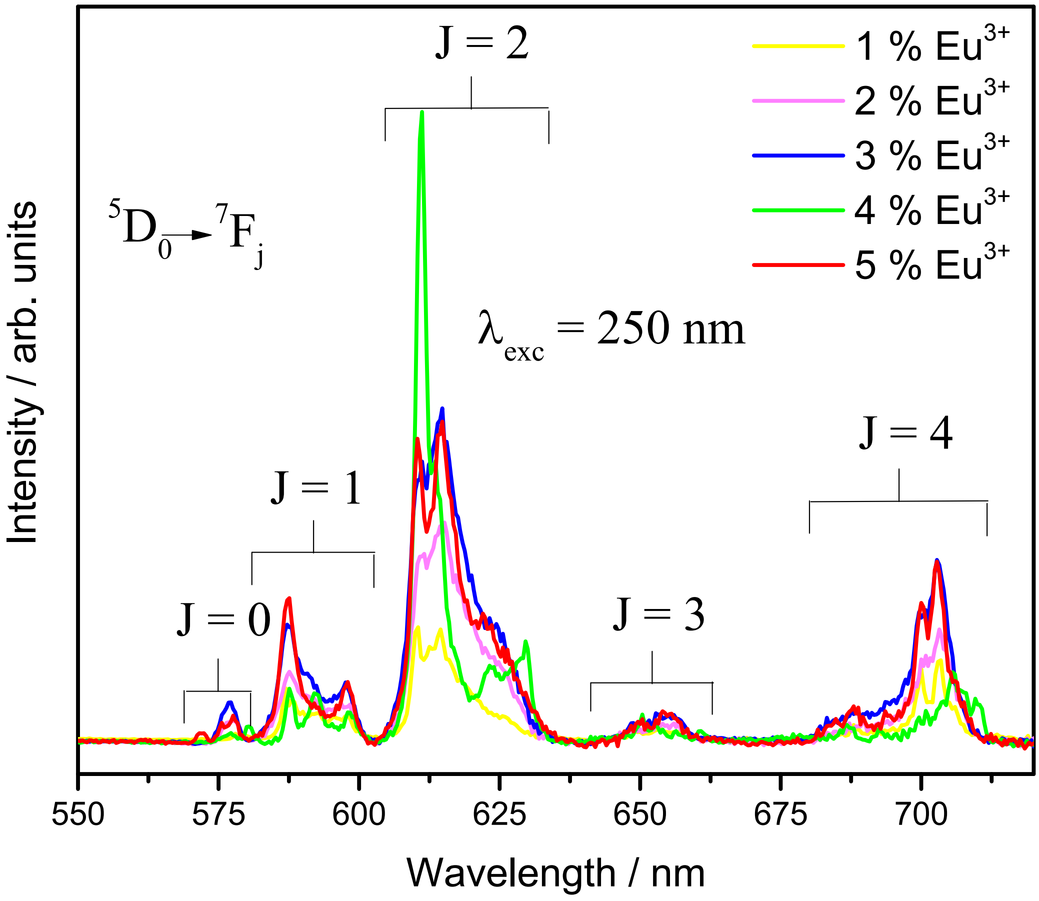


Figure ES7

Figure ES7. Excitation spectra at 77 K of Ba_2SiO_4:Eu^{3+} samples monitoring the Eu^{3+} $^7F_0 \rightarrow {}^5D_0$ transition upon selective emission in the different $^5D_0 \rightarrow {}^7F_2$ components. The lines in the images represents the 0-0 components attributed to Eu^{3+} ions replacing Ba^{2+} ions in the Ba_2SiO_4 network. In the 5 % doped sample, is not possible to see the 0-0 component for the Eu^{3+}-O^{2-} associate probably because the 0-2 lines is very week, since it is governed by a different transition mechanism.

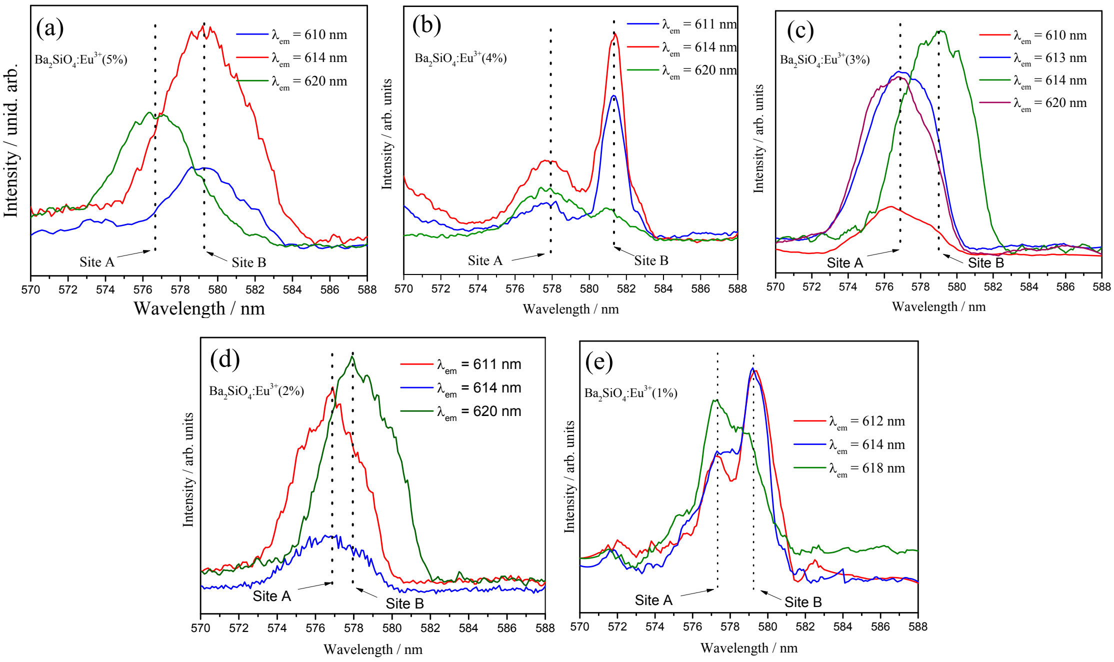


Figure ES8

Figure ES8. (a) Luminescence decay curves fixing excitation wavelength at 394 nm ($^7F_0\rightarrow{}^5L_6$) and emission wavelength at 614 nm ($^5D_0\rightarrow{}^7F_2$), and (b) *ln* of intensity, for all $Ba_2SiO_4:Eu^{3+}$ samples.

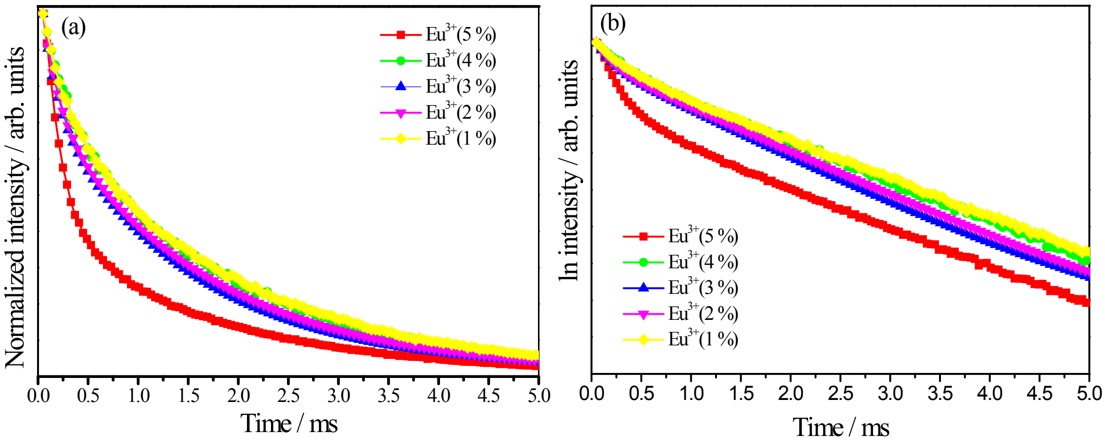
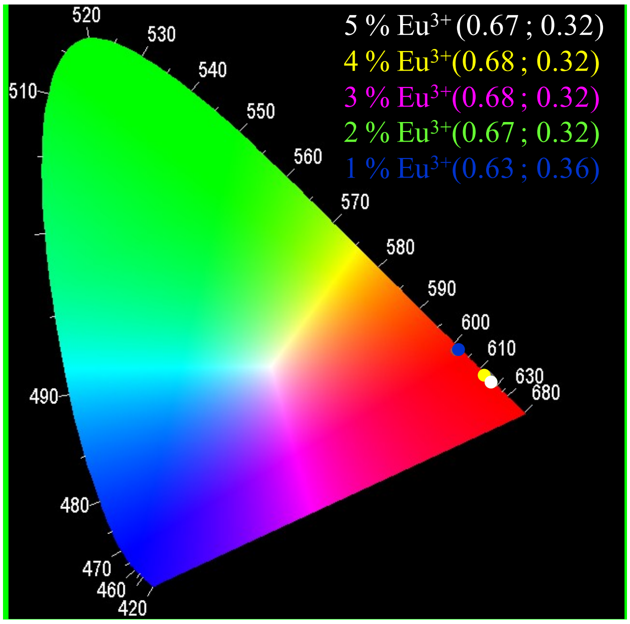


Figure ES9

Figure ES9. CIE chromaticity diagram for $Ba_2SiO_4:Eu^{3+}$(1-5) obtained from Spectra Lux software[2], and the emission spectra collected under 250 nm excitation measured at room temperature.



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[1] A. L. Patterson, *Phys. Rev.,* **56**, 1939, 978.

[2] P.A. Santa-cruz, F.S. Teles. Spectra Lux Software. Versão 2.0 RENAMI, U. Federal de Pernambuco, 2003.