

Supplementary Material

Unveiling the Role of the Hexagonal Polymorph on SrAl₂O₄-based Phosphors

Rocío Estefanía Rojas-Hernandez^{*, †, ‖} , Fernando Rubio-Marcos[†], Aida Serrano[‡], Aydar

Rakhmatullin[§], Catherine Bessada[§], José Francisco Fernandez[†]

[†] *Electroceramic Department, Instituto de Cerámica y Vidrio, CSIC, Kelsen 5, 28049, Madrid, Spain.*

[‖] *Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa
Av. Rovisco Pais, 1049-001 Lisboa, Portugal*

[‡] *SpLine, Spanish CRG Beamline at the ESRF, F-38043 Grenoble, Cedex 09 France and Instituto de Ciencia de Materiales de Madrid, CSIC,*

Cantoblanco, 28049, Madrid, Spain

[§] *CNRS, CEMHTI UPR3079, Univ. Orléans, F-45071 Orléans, France*

Supplementary Information 1:

Figure S1 exhibits the calculated lattice cell parameters and cell volume as a function of ZnO content ((1.25, 2.5, 3.75 and 5% (in weight)) for the $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ (SAO) powders synthesized at 1000 °C for 2 h in 90N₂-10H₂ atmosphere, using a salt/ SrAl_2O_4 molar ratio of 3:1 and $\gamma\text{-Al}_2\text{O}_3$ /SrO ratio of 2.

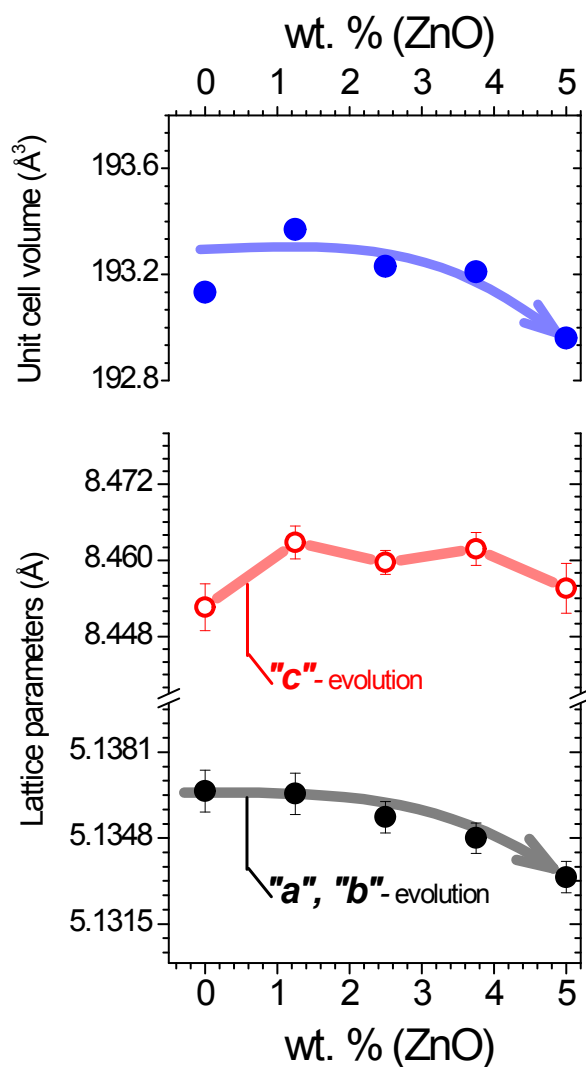


Figure S1. Lattice cell parameters and crystal unit cell volume as a function of ZnO content: From synthesized $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ (SAO) phosphor at 1000 °C for 2 h in 90N₂-10H₂ atmosphere, using a salt/ SrAl_2O_4 molar ratio of 3:1 and $\gamma\text{-Al}_2\text{O}_3$ /SrO ratio of 2 with different ZnO content (1.25, 2.5, 3.75 and 5% (in weight)).

Supplementary Information 2:

Figure S2(a) shows the XRD of the synthesized powder heated at 1000 °C for 2 h in 90N₂-10H₂ atmosphere, employing a salt/SrAl₂O₄ molar ratio of 3:1, a Al₂O₃ /SrO ratio of 2, and as alumina precursor γ -Al₂O₃ with 10% of ZnO. Here it is essential to note that the non-stoichiometric ratio promotes the formation of the hexagonal phase and 10 % of ZnO promotes the secondary phase, Sr₃Al₂O₆. **Figure S1(b)** illustrates the emission spectra of samples with different ZnO contents; showing that the emission intensity decreases with ZnO contents higher than 5 %.

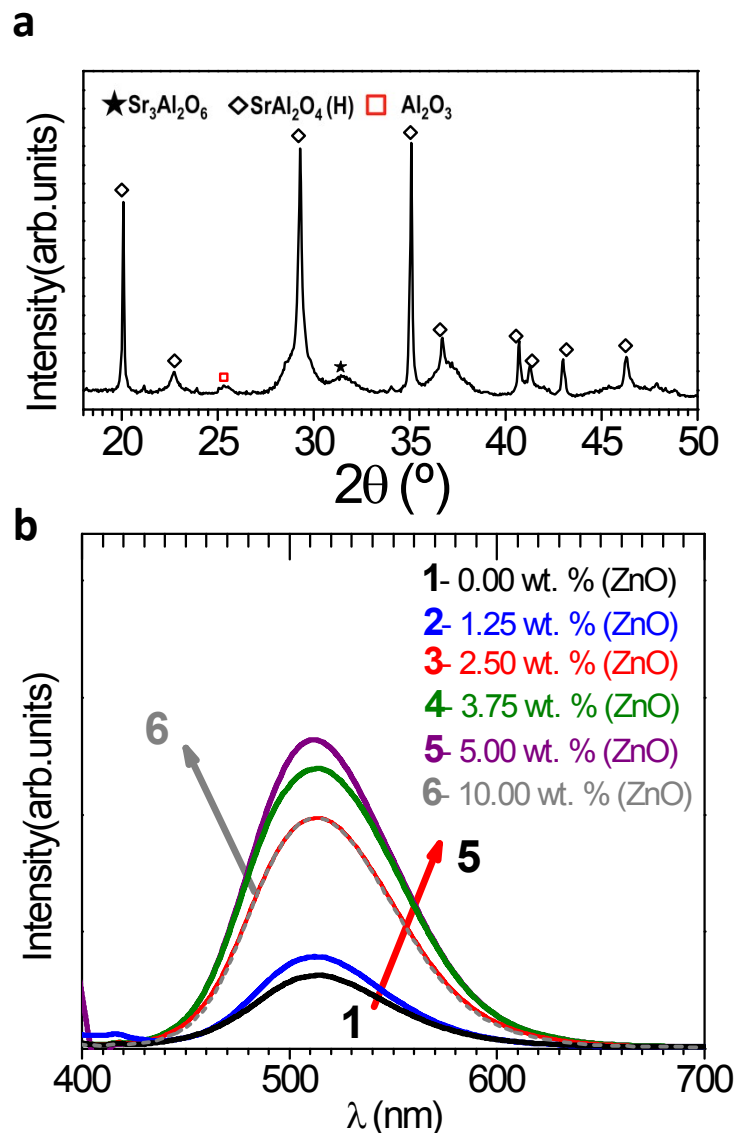


Figure S2. (a) XRD of synthesized SrAl₂O₄:Eu, Dy (SAO) phosphor heated at 1000 °C for 2 h in 90N₂-10H₂ atmosphere, employing a salt/SrAl₂O₄ molar ratio of 3:1, a Al₂O₃ /SrO ratio of 2, and as alumina precursor γ -Al₂O₃ with 10% of ZnO. The symbols highlight SrAl₂O₄ Hexagonal phase (black-open diamonds), Sr₃Al₂O₆ phase (black starts) and Al₂O₃ phase (red-open squares). **(b)** Emission spectra upon excitation at 380 nm of synthesized SrAl₂O₄:Eu, Dy as a function of ZnO incorporation.

Supplementary Information 3:

The chemical composition of the powder synthesized $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ without ZnO (Areas 1, 2, 3, 4 and 5) and with 5 wt. % of ZnO (Areas 6 and 7) was determined by an INCA x-sight energy dispersive X-ray spectrometer (EDXS, Oxford Instruments) which is coupled with the FE-SEM.

Analyzed compositions of the areas from micrographs in **Fig. 4 (a-h)** presented in the main manuscript are summarized in **Table S1**.

Table S1. Elemental analysis from $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ powder synthesized without and with 5 wt. % of ZnO. * Al^{+3} cation excess (Al_2O_3)						
Samples	Sr Atomic %	Al Atomic %	O Atomic %	Eu Atomic %	Dy Atomic %	Zn Atomic %
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ Stoichiometric	13.9	28.6	57.1	0.3	0.1	-
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ + Al_2O_3^*	8.1	33.3	58.3	0.2	0.1	-
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ + Al_2O_3^* + 5% ZnO	8.0	33.1	58.1	0.2	0.1	0.4
Area 1	9.0	32.7	58.2	0.2	0.0	-
Area 2	9.5	32.1	58.1	0.2	0.1	-
Area 3	9.5	32.0	58.1	0.3	0.0	-
Area 4	9.0	32.1	58.2	0.6	0.0	-
Area 5	9.5	32.1	58.1	0.2	0.1	-
Area 6	11.9	29.0	57.4	0.4	0.1	1.3
Area 7	9.6	29.7	57.5	0.2	0.0	3.0

Supplementary Information 4:

The chemical composition of the powder synthesized $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ without ZnO (Point 1 and 2) and with 5wt. % of ZnO (Point 1') was determined by an INCA x-sight energy dispersive X-ray spectrometer (EDXS, Oxford Instruments) which is coupled with the FE-SEM.

Analyzed Compositions of the points from micrographs in **Fig. 5** and **6** presented in the main manuscript are summarized in **Table S2**.

Table S2. Elemental analysis from $\text{SrAl}_2\text{O}_4\text{:Eu, Dy}$ powder synthesized without and with 5% of ZnO. * Al^{+3} cation excess (Al_2O_3)						
Samples	Sr Atomic %	Al Atomic %	O Atomic %	Eu Atomic %	Dy Atomic %	Zn Atomic %
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ Theoretical Stoichiometric	13.9	28.6	57.1	0.3	0.1	-
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ + Al_2O_3^*	8.1	33.3	58.3	0.2	0.1	-
$\text{SrAl}_2\text{O}_4\text{:Eu,Dy}$ + Al_2O_3^* + 5% ZnO	8.0	33.1	58.1	0.2	0.1	0.4
Point 1	6.1	60.0	33.8	0.0	0.0	-
Point 2	0.9	36.1	62.5	0.0	0.0	-
Point 1'	8.1	33.9	58.0	0.0	0.0	0.0