Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Emission colour tuning through coupled N/La introduction in Sr_2SiO_4: Eu^{2+}

Ashley P. Black, Kristin A. Denault, , Carlos Frontera, Ram Sheshadri , Alejandro R. Goñi, and Amparo Fuertes

Supplementary Information

Table S1. Crystallographic and refinement data from synchrotron X-ray powder diffraction data (λ=0.458996 Å, T=298 K) for $Sr_{2-x}La_xSiO_{4-x}N_x$ (x= 0.0, 0.2, 0.3, 0.5, 1.0) .

	β-Sr_2SiO_4	**$La_{0.2}Sr_{1.8}SiO_{3.8}N_{0.2}$**	**$La_{0.3}Sr_{1.7}SiO_{3.7}N_{0.3}$**	**$La_{0.5}Sr_{1.5}SiO_{3.5}N_{0.5}$**	**$LaSrSiO_3N$**
Space group	$P2_1/n$	Pmnb	Pmnb	Pmnb	Pmnb
a(Å)	5.6613(1)	5.65855(1)	5.6545(1)	5.6523(1)	5.64986(5)
b(Å)	7.0808(1)	7.0942(1)	7.1014(1)	7.1100(1)	7.11547(5)
c(Å)	9.7558(1)	9.7591(2)	9.7641(2)	9.7778(2)	9.8172(1)
β(º)	92.6515(8)				
V(Å^3)	390.66(1)	391.76(1)	392.08(1)	392.95(1)	394.67(1)
N_p, N_{irefl} [(a)]	34500, 2617	34500, 1394	34500, 1403	34500, 1400	34500, 1435
P_p, P_i, P_g [(b)]	17, 63, 7	13, 24, 39	15, 24, 6	15, 29, 7	13, 26, 7
R_{Bragg}, R_f, χ^2	5.0, 3.0, 1.43	4.16, 5.06, 1.38	4.88, 4.81, 2.01	4.15, 3.6, 2.70	3.43, 3.88, 1.37
R_p, R_{wp}, R_{ex} [(c)]	9.20, 13.6, 11.34	9.51, 13.0, 11.13	8.98, 13.3, 9.45	9.79, 14.4, 8.73	5.98, 9.38, 8.02

(a) N_p, N_{irefl} refer to the number of experimental points and independent reflections.

(b) P_p, P_i, P_g, refer to the number of profile, intensity-affecting and global refined parameters, respectively.

(c) Conventional Rietveld R-factors (R_p, R_{wp} , R_{exp}) in %

Table S2. Atomic coordinates, cation and anion occupancies for $Sr_{1.5}La_{0.5}SiO_{3.5}N_{0.5}$ [(a,b)]

Site	**Wyckoff position**	**x**	**y**	**z**	**occupation factor**
La1/Sr1	4c	0.25	0.6575(7)	0.4175(3)	0.054(9)/0.946
La2/Sr2	4c	0.25	0.0055(7)	0.42182(6)	0.446/0.554
Si	4c	0.25	0.221(2)	0.6966(5)	1
O1/N1	4c	0.25	0.9950(5)	0.4343(4)	1/0
O2/N2	4c	0.25	0.331(8)	0.570(5)	0.5/0.5
O3/N3	8d	0.012(5)	0.286(4)	0.338(4)	0.75/0.25

(a) Estimated standard deviations in parentheses are shown once for each independent variable. La/Sr occupation factors were refined subject to the ideal stoichiometry. O/N occupation factors were considered fixed to those obtained in $LaBaSiO_3N$ from neutron diffraction in A. P. Black, K. A. Denault, J. Oro-Sole, A. R. Goñi and A. Fuertes, Chem. Comm., 2015, 51, 2166.

(b) Refined isotropic B-factors were 0.83(3) Å^2 for silicon, 2.06(9) Å^2 for O2/N2 and 1.74(7) Å^2 for O3/N3. Temperature factors were refined anisotropically for La/Sr and O1/N1. Resulting equivalent B-factors were 1.29 Å^2, 0.99 Å^2 and 2.95 Å^2 for La1/Sr1, La2/Sr2 and O1/N1, respectively.

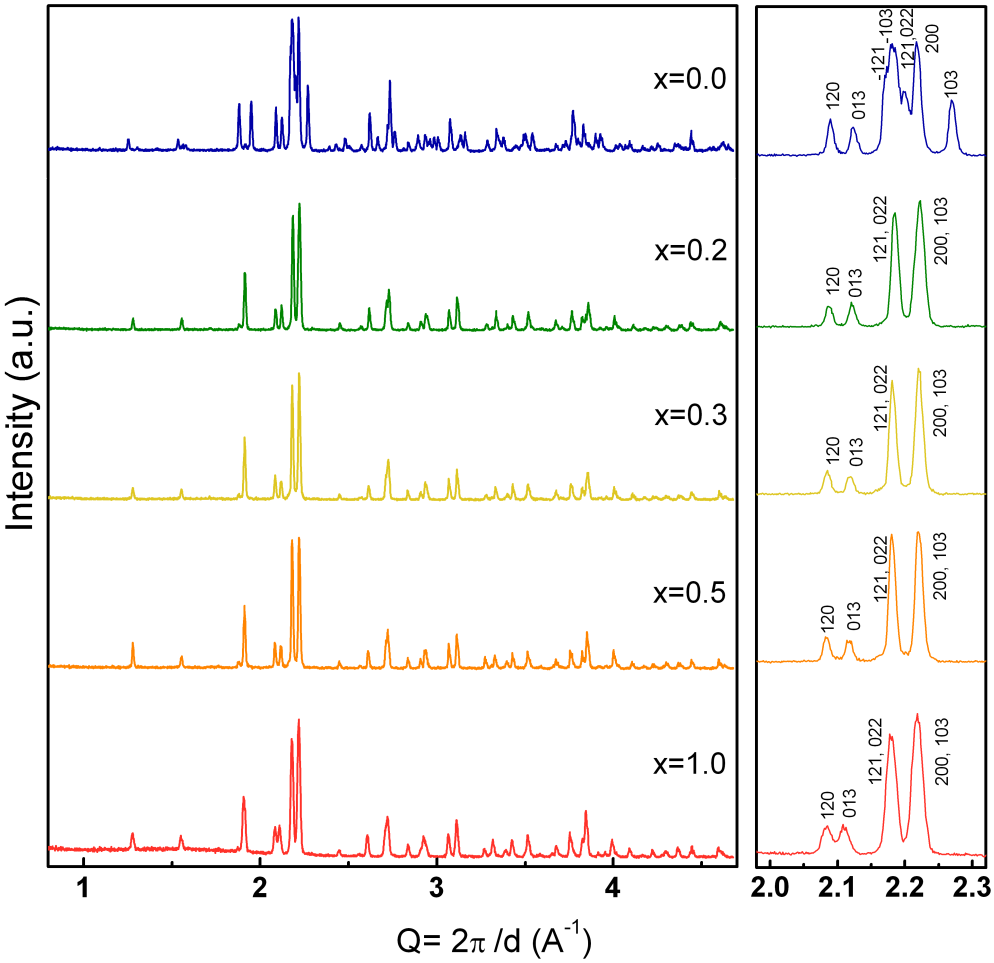

Figure S1. X-ray powder diffraction patterns for $Sr_{1.98-x}Eu_{0.02}La_xSiO_{4-x}N_x$ ($0 \geq x \geq 1$) and enlarged images of the intense reflections around Q=2 Å $^{-1}$ region.

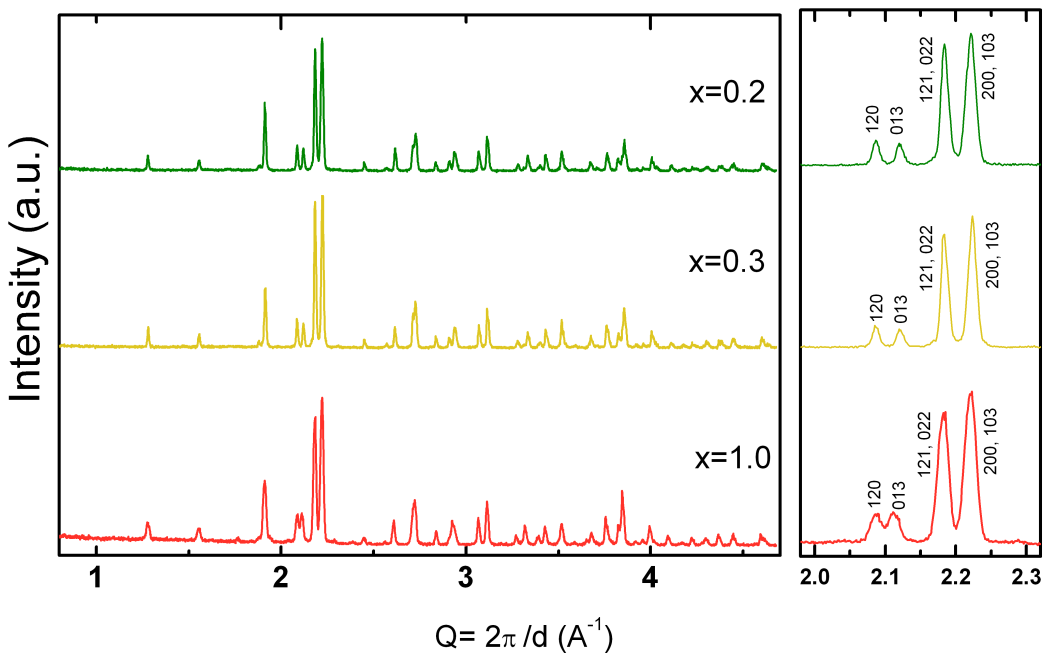

Figure S2. X-ray powder diffraction patterns for $Sr_{2-x}La_{x-0.02}Ce_{0.02}SiO_{4-x}N_x$ (0.2, 0.3, 1.0) and enlarged images of the intense reflections around Q=2 Å $^{-1}$ region.

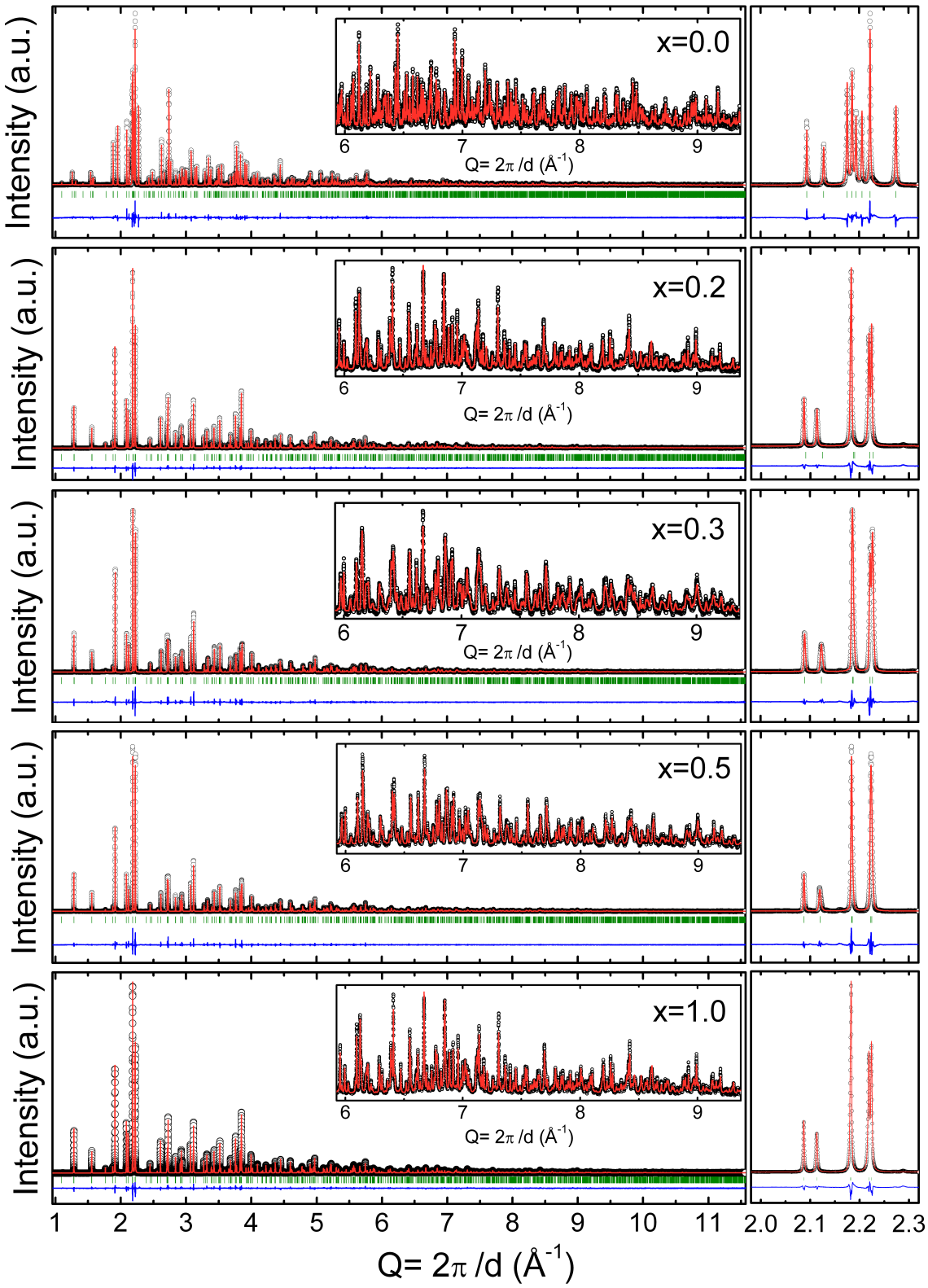

Figure S3. Observed and calculated synchrotron X-ray powder diffraction patterns for $Sr_{2-x}La_xSiO_{4-x}N_x$.

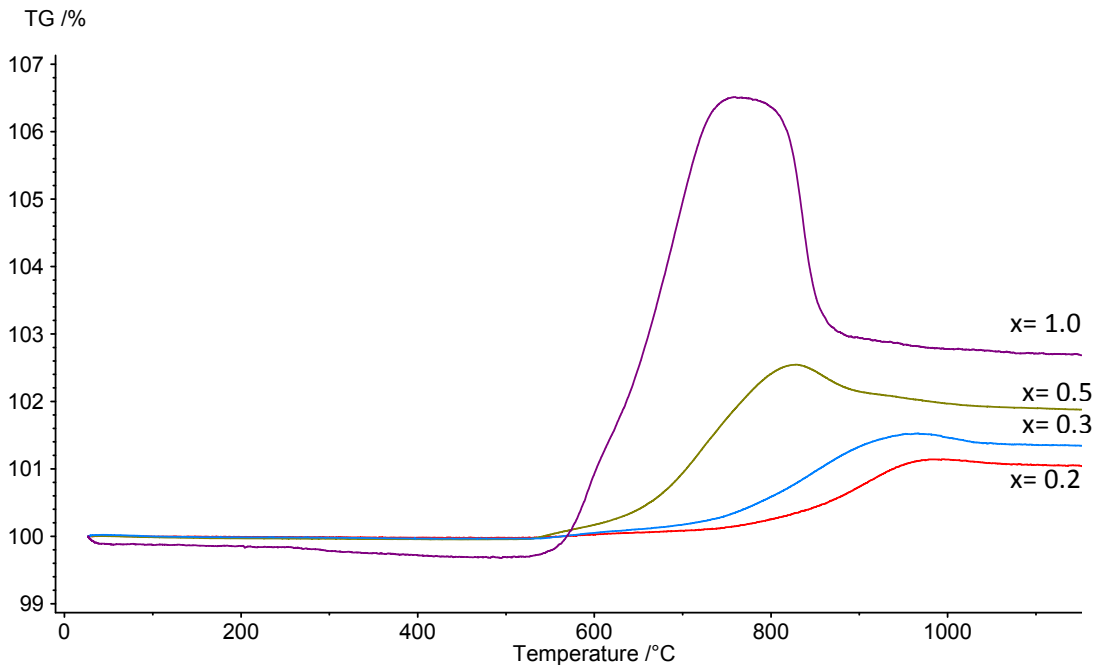

Figure S4. TGA curves in O_2 for $Sr_{2-x}La_xSiO_{4-x}N_x$.

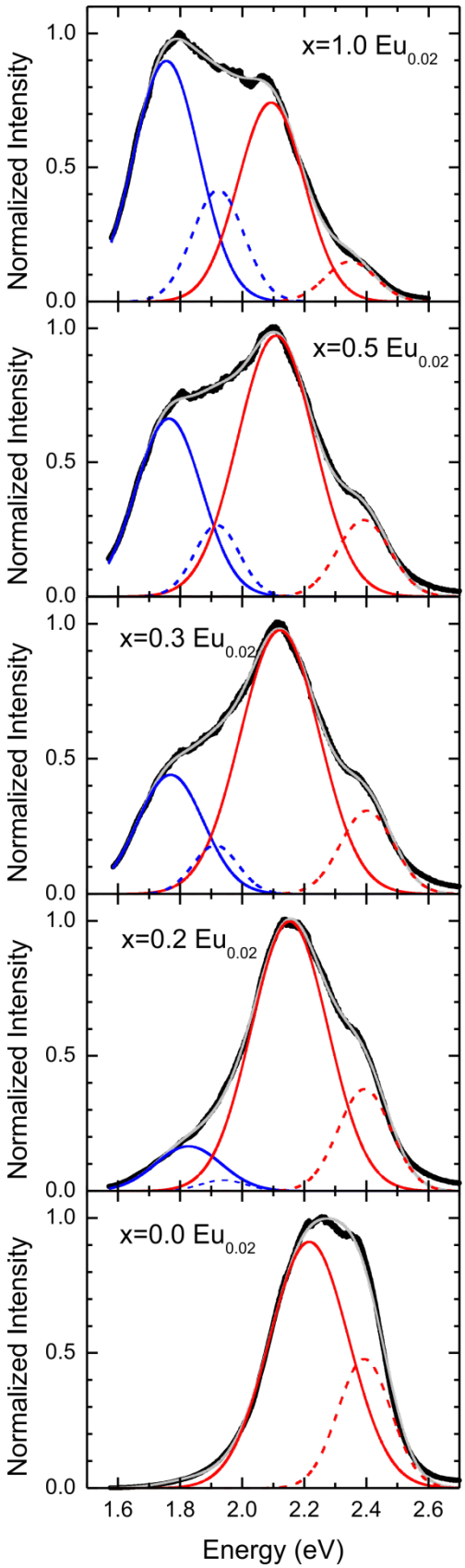

Figure S5. Deconvolution of emission spectra of $Sr_{2-x}La_xSiO_{4-x}N_x:Eu_{0.02}$ under excitation at 405 nm.

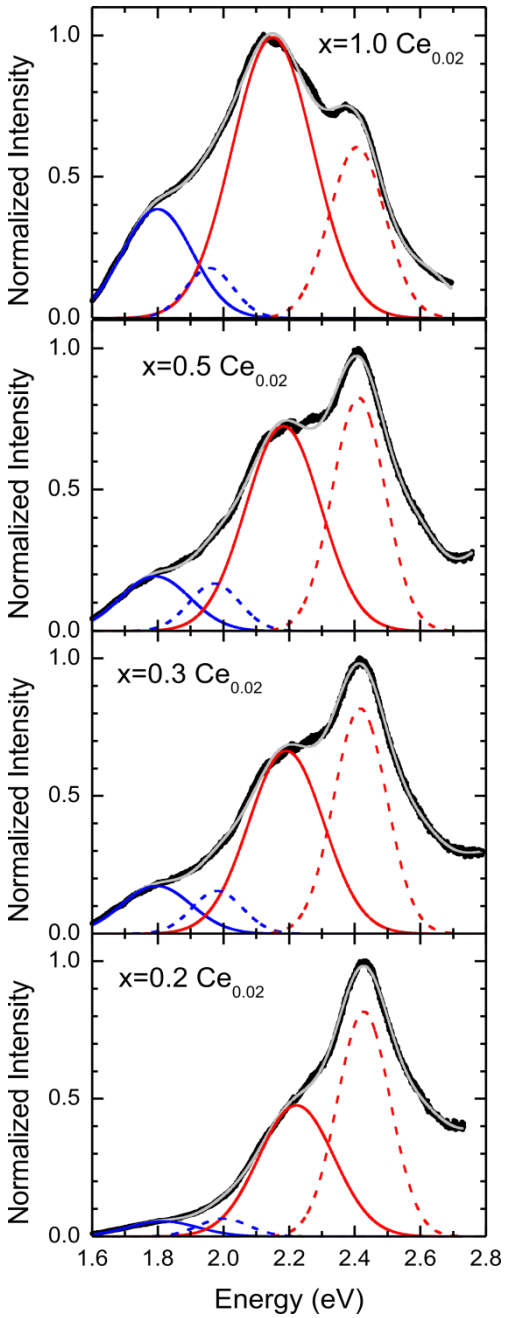

Figure S6. Deconvolution of emission spectra of $Sr_{2-x}La_xSiO_{4-x}N_x:Ce_{0.02}$ under excitation at 405 nm.