Electronic Supplementary Information for

B-site ordered double perovskite $LaBa_{1-x}Sr_xZnSbO_6$ ($0 \leq x \leq 1$): Sr^{2+}-doping-induced symmetry evolution and structure-luminescence correlations

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Table S1 Lattice parameters of Eu^{3+} doped samples obtained by Le-Bail fitting.

Formula	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)	*β* (°)
$La_{0.95}Eu_{0.05}BaZnSbO_6$	5.7093	5.7092	8.0735	263.16	89.893
$La_{0.95}Eu_{0.05}Ba_{0.8}Sr_{0.2}ZnSbO_6$	5.6977	5.6943	8.0576	261.42	90.138
$La_{0.95}Eu_{0.05}Ba_{0.6}Sr_{0.4}ZnSbO_6$	5.6908	5.6850	8.0632	260.86	90.219
$La_{0.95}Eu_{0.05}Ba_{0.4}Sr_{0.6}ZnSbO_6$	5.6798	5.6740	8.0276	258.71	90.011
$La_{0.95}Eu_{0.05}Ba_{0.2}Sr_{0.8}ZnSbO_6$	5.6739	5.6702	8.0219	258.08	90.040
$La_{0.975}Eu_{0.025}SrZnSbO_6$	5.6564	5.6567	7.9991	255.94	89.976
$La_{0.95}Eu_{0.05}SrZnSbO_6$	5.6566	5.6569	7.9977	255.92	89.995
$La_{0.92}Eu_{0.08}SrZnSbO_6$	5.6537	5.6552	7.9941	255.59	90.006

Table S2 Atomic coordinates, isotropic thermal displacement factors and site occupancies for $LaBa_{1-x}Sr_xZnSbO_6$ (x = 0.2, 0.4, 0.6, 0.8).

$LaBa_{0.8}Sr_{0.2}ZnSbO_6$	*x*	*y*	*z*	Occupancy	B_{eq} (Å^2)
Ba/La/Sr	0.499(1)	0	0.2495(4)	0.4/0.5/0.1	0.014(1)
Zn	0	0	0	1	0.014(1)
Sb	0	0	0.5	1	00.011(3)
O1	0.063(2)	0	0.256(3)	1	0.018(1)
O2	0.275(2)	0.236(2)	0.971(1)	1	0.018(1)
$LaBa_{0.6}Sr_{0.4}ZnSbO_6$	*x*	*y*	*z*	Occupancy	B_{eq} (Å^2)
Ba/La/Sr	0.498(1)	0	0.2492(3)	0.3/0.5/0.2	0.014(1)
Zn	0	0	0	1	0.014(1)
Sb	0	0	0.5	1	0.011(1)
O1	0.066(2)	0	0.251(3)	1	0.022(1)
O2	0.264(3)	0.246(2)	0.031(1)	1	0.022(1)
$LaBa_{0.4}Sr_{0.6}ZnSbO_6$	*x*	*y*	*z*	Occupancy	B_{eq} (Å^2)

Ba/La/Sr	0.001(1)	0.5140(3)	0.2519(7)	0.2/0.5/0.3	0.009(1)
Zn	0	0	0	1	0.005(1)
Sb	0	0	0.5	1	0.003(1)
O1	0.081(4)	0.991(3)	0.262(5)	1	0.005(3)
O2	0.759(6)	0.275(5)	0.007(4)	1	0.005(3)
O3	0.277(5)	0.231(5)	0.954(3)	1	0.005(3)

$LaBa_{0.2}Sr_{0.8}ZnSbO_6$	*x*	*y*	*z*	Occupancy	B_{eq} (Å^2)
Ba/La/Sr	0.005(2)	0.5202(2)	0.253(1)	0.1/0.5/0.4	0.008(1)
Zn	0	0	0	1	0.006(1)
Sb	0	0	0.5	1	0.0043(9)
O1	0.090(3)	0.995(2)	0.253(4)	1	0.003(2)
O2	0.759(5)	0.272(4)	0.005(3)	1	0.003(2)
O3	0.293(4)	0.228(4)	0.954(3)	1	0.003(2)

Table S3 Selected interatomic distances (Å) and bond angles (°) for $LaBa_{1-x}Sr_xZnSbO_6$ (x = 0.2, 0.4, 0.6, 0.8). Calculated bond valence sums (BVS) for Zn^{2+} and Sb^{5+} are also given.

$LaBa_{0.8}Sr_{0.2}ZnSbO_6$			
La/Ba/Sr-O2 ×2	2.61(1)	Zn-O1 ×2	2.11(2)
La/Ba/Sr -O2 ×2	2.79(1)	Zn-O2 ×4	2.08(1)
La/Ba/Sr -O2 ×2	2.94(1)	BVS	2.09
La/Ba/Sr -O2 ×2	3.10(1)	Sb-O1 ×2	1.98(2)
La/Ba/Sr -O1 ×1	2.8(2)	Sb-O2 ×4	1.99(1)
La/Ba/Sr -O1 ×2	2.87(2)	BVS	5.33
La/Ba/Sr -O1 ×1	3.43(2)	Zn-O1- Sb	158.9
		Zn-O2- Sb	165.3

$LaBa_{0.6}Sr_{0.4}ZnSbO_6$

La/Ba/Sr -O2 ×2	2.57(1)	Zn-O1 ×2	2.09(2)
La/Ba/Sr -O2 ×2	2.81(1)	Zn-O2 ×4	2.08(1)
La/Ba/Sr -O2 ×2	2.91(1)	BVS	2.16
La/Ba/Sr -O2 ×2	3.12(1)	Sb-O1 ×2	1.99(2)
La/Ba/Sr -O1 ×1	2.49(2)	Sb-O2 ×4	1.99(1)
La/Ba/Sr -O1 ×2	2.86(2)	BVS	2.25
La/Ba/Sr -O1 ×1	3.23(2)	Zn-O1- Sb	159.7
		Zn-O2- Sb	163.9

$LaBa_{0.4}Sr_{0.6}ZnSbO_6$

La/Ba/Sr-O1	2.39(2)	Zn-O1 ×2	2.15(4)
La/Ba/Sr-O1	2.75(2)	Zn-O2 ×2	2.08(3)
La/Ba/Sr-O1	3.00(2)	Zn-O3 ×2	2.09(3)
La/Ba/Sr-O1	3.31(2)	BVS	2.04
La/Ba/Sr-O2	2.75(3)	Sb-O1 ×2	1.97(4)
La/Ba/Sr-O2	2.76(3)	Sb-O2 ×2	1.95(3)
La/Ba/Sr-O2	2.85(3)	Sb-O3 ×2	2.02(3)
La/Ba/Sr-O2	3.01(3)	BVS	5.44
La/Ba/Sr-O3	2.49(3)	Zn-O1- Sb	154.0
La/Ba/Sr-O3	2.71(3)	Zn-O2- Sb	171.5
La/Ba/Sr-O3	2.95(3)	Zn-O3- Sb	156.8
La/Ba/Sr-O3	3.28(3)		

$LaBa_{0.2}Sr_{0.8}ZnSbO_6$

La/Ba/Sr-O1	2.30(2)	Zn-O1 ×2	2.09(3)
La/Ba/Sr-O1	2.73(2)	Zn-O2 ×2	2.06(3)
La/Ba/Sr-O1	3.02(2)	Zn-O3 ×2	2.14(2)
La/Ba/Sr-O2	2.73(3)	BVS	2.08

La/Ba/Sr-O2	2.80(3)	Sb-O1 ×2	2.04(3)
La/Ba/Sr-O2	2.83(3)	Sb-O2 ×2	1.96(3)
La/Ba/Sr-O2	2.99(3)	Sb-O3 ×2	1.97(2)
La/Ba/Sr-O3	2.46(3)	BVS	5.28
La/Ba/Sr-O3	2.77(3)	Zn-O1- Sb	151.3
La/Ba/Sr-O3	2.87(3)	Zn-O2- Sb	172.4
La/Ba/Sr-O3	3.34(2)	Zn-O3- Sb	154.7

Table S4 Lattice parameters of $LaBa_{1-x}Sr_xZnSbO_6$ ($0 \leq x \leq 1$) obtained by Rietveld refinement.

Formula	a (Å)	b (Å)	c (Å)	V (Å^3)	β (^{o})
$LaBaZnSbO_6$	5.7253(2)	5.7066(3)	8.0689(3)	263.63(2)	90.00(4)
$LaBa_{0.8}Sr_{0.2}ZnSbO_6$	5.7247(1)	5.6960(1)	8.0533(2)	262.602(9)	90.01(1)
$LaBa_{0.6}Sr_{0.4}ZnSbO_6$	5.7132(1)	5.6807(1)	8.0318(2)	260.67(1)	90.035(6)
$LaBa_{0.4}Sr_{0.6}ZnSbO_6$	5.6945(2)	5.6731(2)	8.0225(3)	259.17(2)	89.99(2)
$LaBa_{0.2}Sr_{0.8}ZnSbO_6$	5.6750(2)	5.6667(2)	8.0126(2)	257.67(1)	89.961(6)
$LaSrZnSbO_6$	5.6586(2)	5.6577(2)	7.9964(2)	256.00(2)	90.00(2)

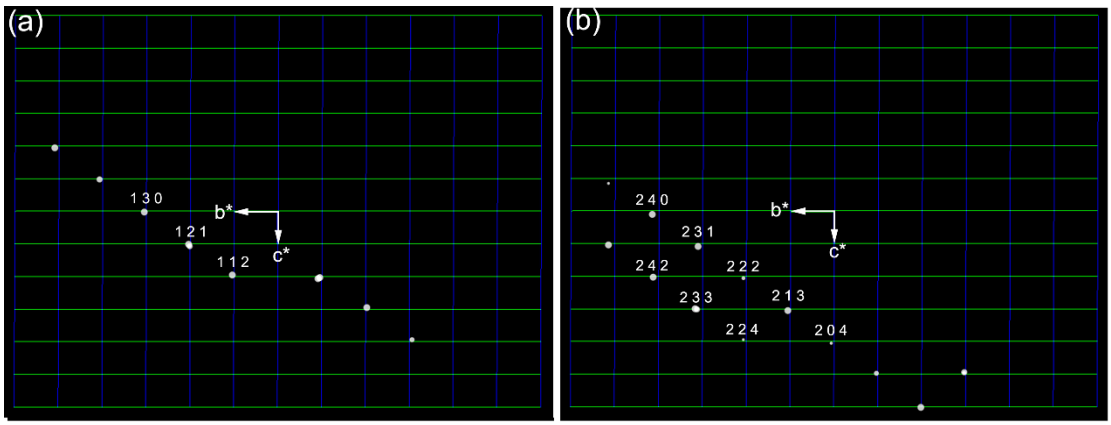


Fig. S1 Selected views in the reciprocal space corresponding to (a) 1*kl* and (b) 2*kl* planes for $LaBaZnSbO_6$. The reflection condition is consistent with $h + k + l = 2n$.

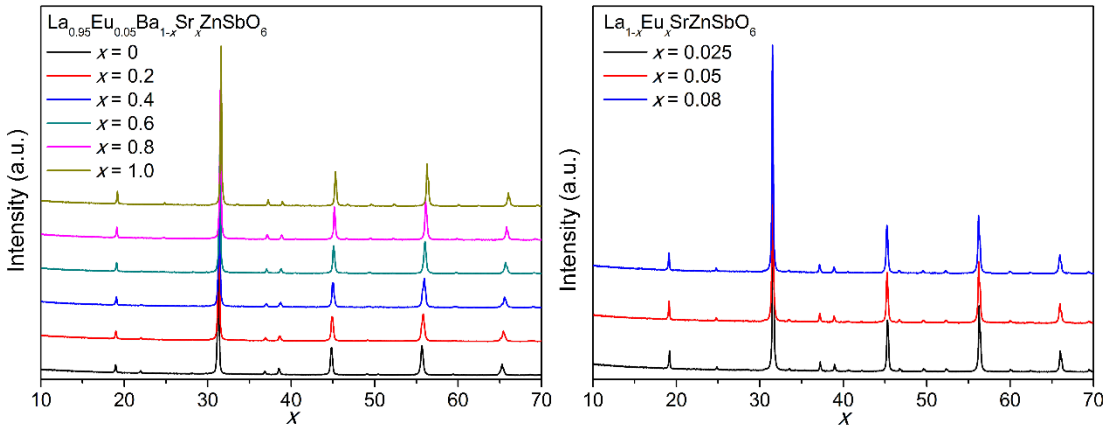
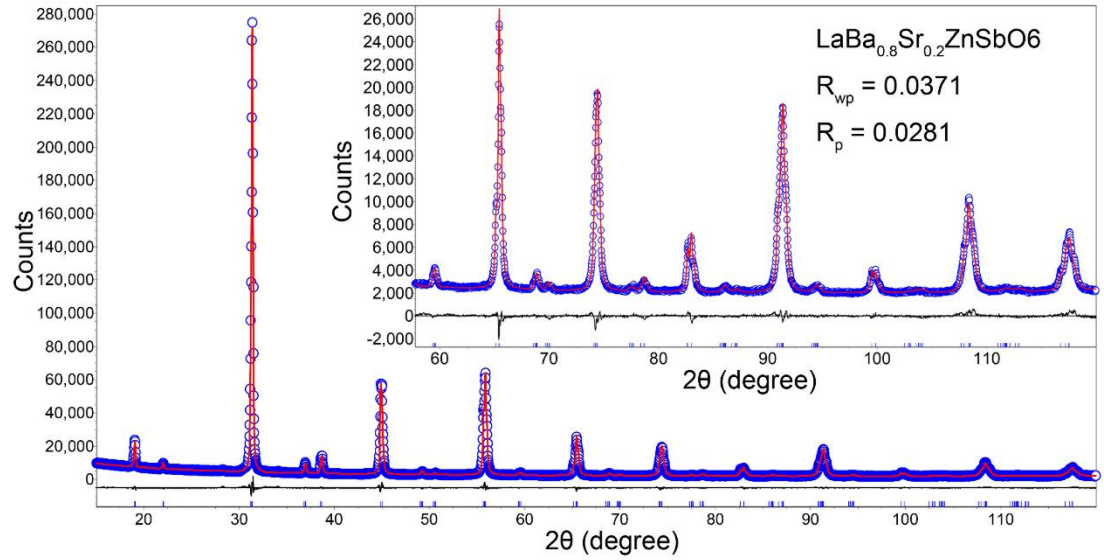
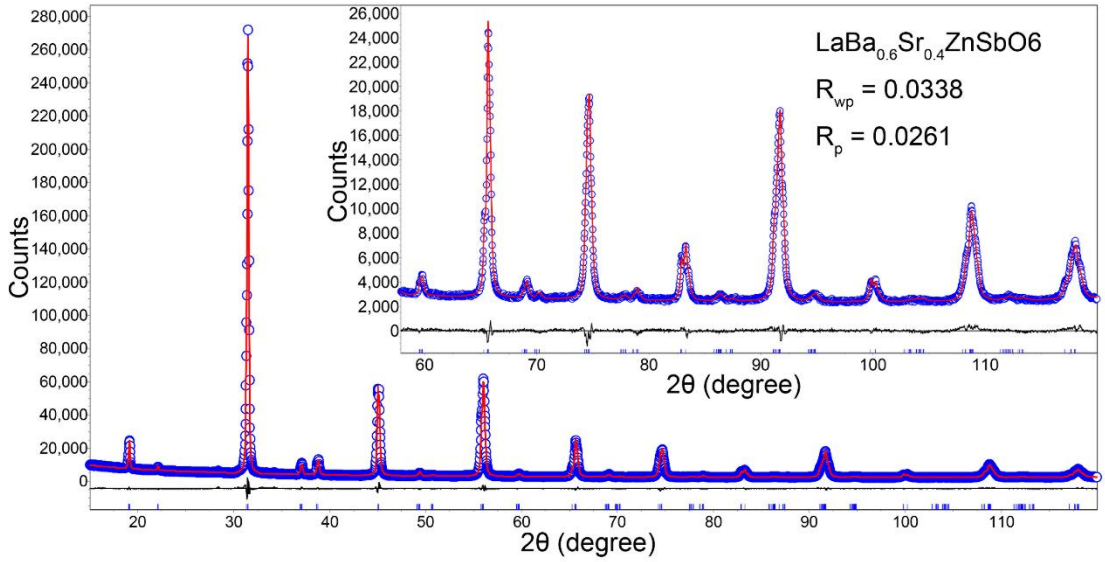


Fig. S2 XRD patterns for $La_{0.95}Eu_{0.05}Ba_{1-x}Sr_xZnSbO_6$ ($0 \leq x \leq 1$) and $La_{1-x}Eu_xSrZnSbO_6$ (x = 0.025, 0.05, 0.08).


LaBa0.8Sr0.2ZnSbO6
Rwp = 0.0371
Rp = 0.0281
Counts
2θ (degree)


LaBa0.6Sr0.4ZnSbO6
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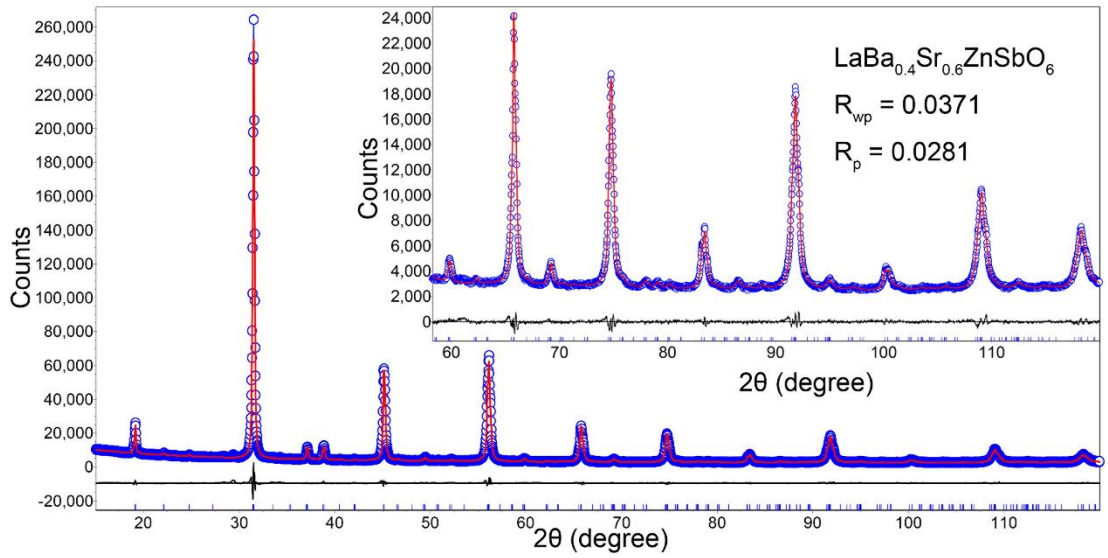
Rp = 0.0261
Counts
2θ (degree)


LaBa0.4Sr0.6ZnSbO6
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Rp = 0.0281
Counts
2θ (degree)

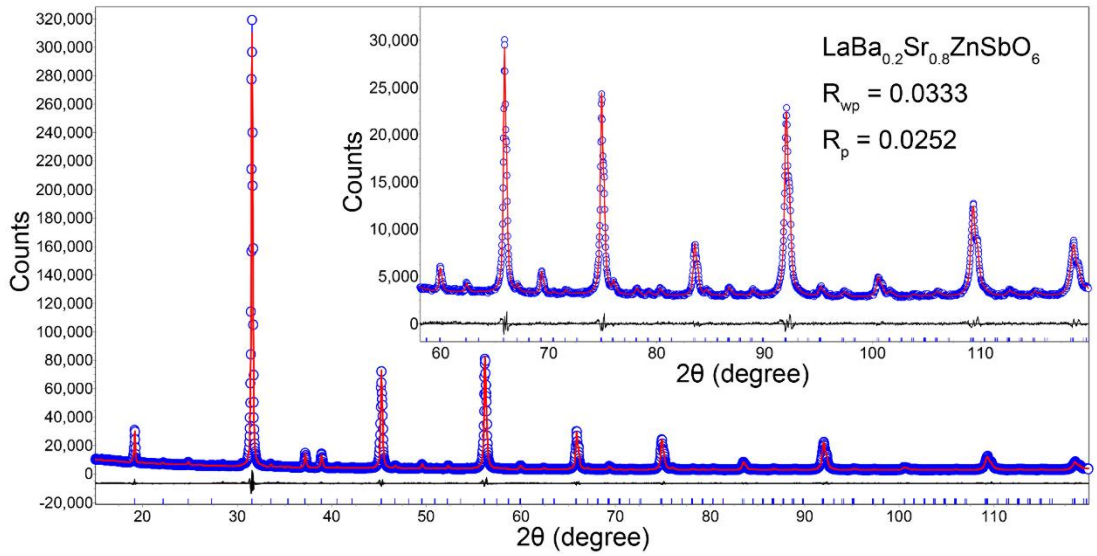

Fig. S3 Final convergence of Rietveld refinement for $LaBa_{1-x}Sr_xZnSbO_6$ (x = 0.2, 0.4, 0.6, 0.8). The blue symbol ○ represents observed data and the red solid line is the calculated pattern; the blue marks below the diffraction patterns are the expected reflection positions, and the difference curve is also shown at the bottom. Enlargements of the high angle part are shown in the top-right corner.

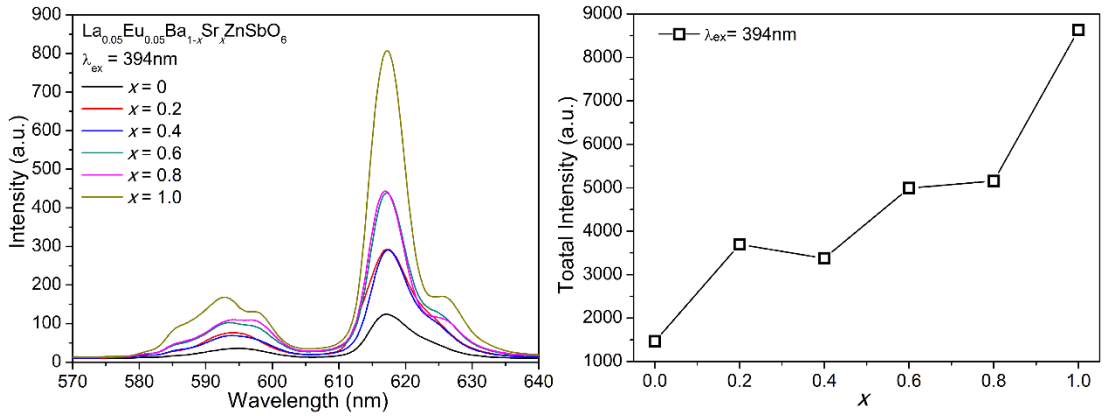

Fig. S4 (a) emission spectra of $La_{0.95}Eu_{0.05}Ba_{1-x}Sr_xZnSbO_6$ excited by 394 nm; (b) total emission intensities excited under 394 nm along with the content of Sr^{3+}.

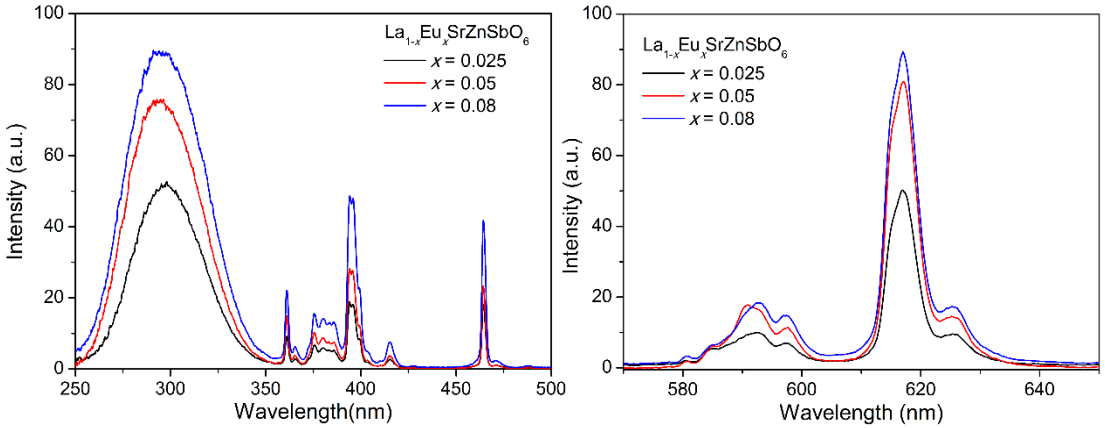

Fig. S5 Excitation (left) and emission (right) spectra for $La_{1-x}Eu_xSrZnSbO_6$ (x = 0.025, 0.05, 0.08).