

**Improvement of thermally stable and photoluminescence in $\text{Sr}_{0.8}\text{Ca}_{0.2}\text{Al}_2\text{Si}_2\text{O}_8:\text{Eu}^{2+}$ by the
substitution of Si-Na # Al-Sr and Ca # Sr on structural modifications**

Zhenling Li, Zhijun Wang*, Panlai Li*, Jinge Cheng, Miaomiao Tian, Chao Wang, Zhiping Yang

Hebei Key Lab of Optic-Electronic Information and Materials, Hebei University, Baoding 071002, China

Table S1 Atomic coordination of $\text{Sr}_{0.8}\text{Ca}_{0.2}\text{Al}_2\text{Si}_2\text{O}_8$

Atom	Position	x	y	z	Occupancy
Ca1	24i	0.2713	-0.0002	0.0665	0.2
Sr1	24i	0.2713	-0.0002	0.0665	0.8
Ca2	24i	0.2702	0.0041	0.5650	0.2
Sr2	24i	0.2702	0.0041	0.5650	0.8
Si1	24i	0.0074	0.1725	0.1079	0.88
Al1	24i	0.0074	0.1725	0.1079	0.12
Si2	24i	0.0027	0.1762	0.6158	0.12
Al2	24i	0.0027	0.1762	0.6158	0.88
Si3	24i	0.0024	0.8205	0.1168	0.12
Al3	24i	0.0024	0.8205	0.1168	0.88
Si4	24i	0.0073	0.8234	0.6090	0.88
Al4	24i	0.0073	0.8234	0.6090	0.12
Si5	24i	0.6945	0.1197	0.1691	0.12
Al5	24i	0.6945	0.1197	0.1691	0.88
Si6	24i	0.6846	0.1123	0.6700	0.88
Al6	24i	0.6846	0.1123	0.6700	0.12
Si7	24i	0.6862	0.8860	0.1740	0.88
Al7	24i	0.6862	0.8860	0.1740	0.12
Si8	24i	0.6942	0.8786	0.6717	0.12
Al8	24i	0.6942	0.8786	0.6717	0.88

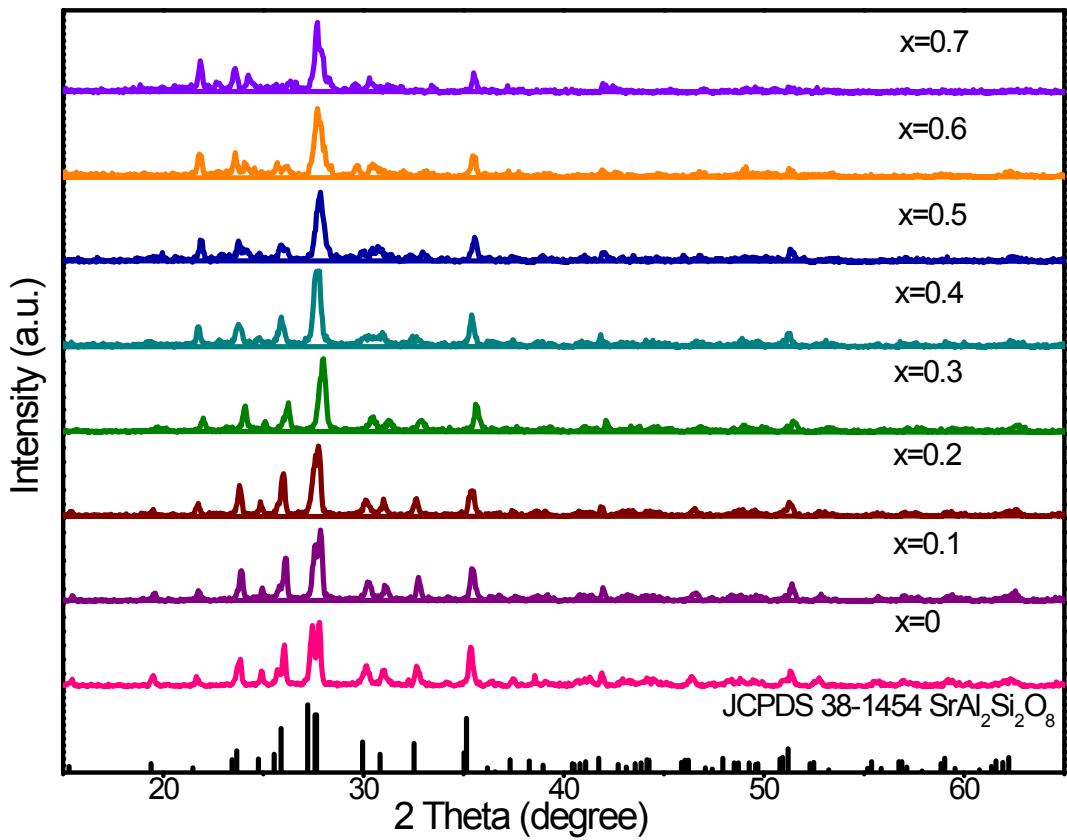


Fig.S1 XRD patterns of $\text{Sr}_{0.77-x}\text{Na}_x\text{Ca}_{0.2}\text{Al}_{2-x}\text{Si}_{2+x}\text{O}_8:0.03\text{Eu}^{2+}$ ($x=0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ and 0.7).

TableS2 Atomic fraction, coordinates and isotropic displacement parameters for $\text{Sr}_{0.77-x}\text{Na}_x\text{Ca}_{0.2}\text{Al}_{2-x}\text{Si}_{2+x}\text{O}_8:0.03\text{Eu}^{2+}$ series. ($x=0, 0.2, 0.4, 0.6$)

x	Atom	Fraction	x	y	z	Uiso
0	Ca1	0.2412	0.2713	-0.0002	0.0665	0.1337
	Sr1	0.7299	0.2713	-0.0002	0.0665	0.1337
	Eu1	0.0289	0.2713	-0.0002	0.0665	0.09
	Ca2	0.1588	0.2702	0.0041	0.5650	0.0032
	Sr2	0.8101	0.2702	0.0041	0.5650	0.06652
	Eu2	0.0311	0.2702	0.0041	0.5650	0.025
0.2	Ca1	0.2364	0.2713	-0.0002	0.0665	0.00946
	Sr1	0.7345	0.2713	-0.0002	0.0665	0.00946
	Eu1	0.0291	0.2713	-0.0002	0.0665	0.025
	Ca2	0.1741	0.2702	0.0041	0.5650	0.00426
	Sr2	0.795	0.2702	0.0041	0.5650	0.00426
	Eu2	0.0309	0.2702	0.0041	0.5650	0.025
0.4	Ca1	0.2257	0.2713	-0.0002	0.0665	0.03062
	Sr1	0.7446	0.2713	-0.0002	0.0665	0.03062
	Eu1	0.0297	0.2713	-0.0002	0.0665	0.025
	Ca2	0.1703	0.2702	0.0041	0.5650	0.042
	Sr2	0.7994	0.2702	0.0041	0.5650	0.042
	Eu2	0.0303	0.2702	0.0041	0.5650	0.025
0.6	Ca1	0.2135	0.2713	-0.0002	0.0665	0.0032
	Sr1	0.7651	0.2713	-0.0002	0.0665	0.01753
	Eu1	0.0214	0.2713	-0.0002	0.0665	0.01753
	Ca2	0.1692	0.2702	0.0041	0.5650	0.0032
	Sr2	0.7922	0.2702	0.0041	0.5650	0.14579
	Eu2	0.0386	0.2702	0.0041	0.5650	0.17048

Table S3 Bond length (Å) of $\text{Sr}_{0.77-x}\text{Na}_x\text{Ca}_{0.2}\text{Al}_{2-x}\text{Si}_{2+x}\text{O}_8:0.03\text{Eu}^{2+}$ ($x=0, 0.2, 0.4, 0.6$)

(EuO)6	x=0	x=0.2	x=0.4	x=0.6
Eu-O3	2.428	2.406	2.397	2.383
Eu-O15	2.801	2.802	2.803	2.829
Eu-O13	2.732	2.724	2.723	2.712
Eu-O1	2.678	2.658	2.652	2.624
Eu-O1	2.627	2.611	2.608	2.619
Eu-O5	2.725	2.717	2.712	2.679
d_{ave}	2.665	2.653	2.65	2.641
D	0.0344	0.0363	0.0372	0.0375
(EuO)7	x=0	x=0.2	x=0.4	x=0.6
O8	2.781	2.773	2.782	2.824
O6	2.828	2.82	2.816	2.78
O2	2.651	2.635	2.627	2.598
O2	2.652	2.636	2.631	2.644
O14	2.701	2.695	2.693	2.672
O16	2.859	2.851	2.86	2.893
O4	2.432	2.412	2.401	2.388
d_{ave}	2.701	2.689	2.687	2.686
D	0.0388	0.0408	0.0428	0.0468

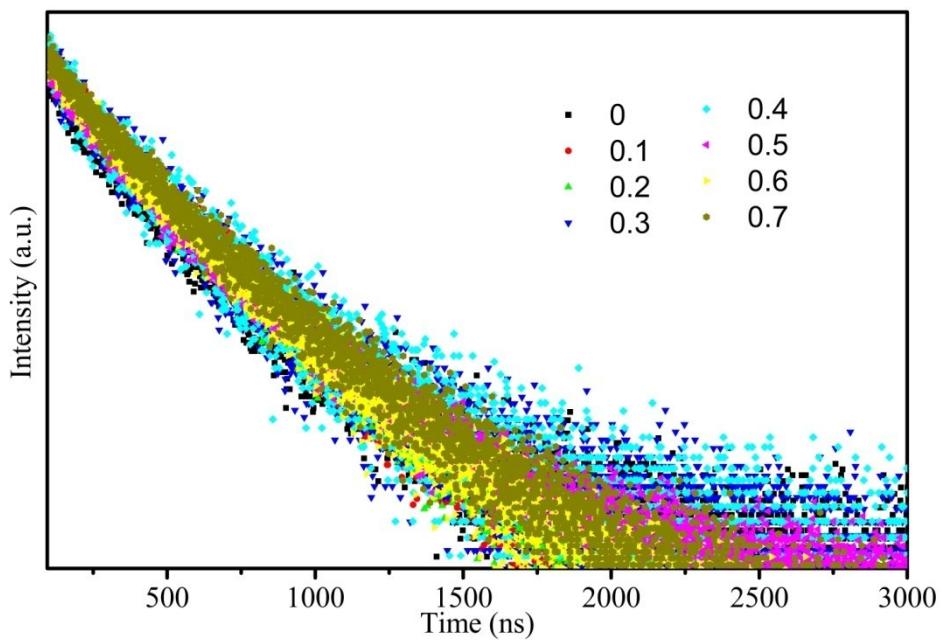


Fig.S2 Decay curves of $\text{Sr}_{0.77-x}\text{Na}_x\text{Ca}_{0.2}\text{Al}_{2-x}\text{Si}_{2+x}\text{O}_8:0.03\text{Eu}^{2+}$ ($x=0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ and 0.7) samples at room temperature.

Table S4 The life times of Eu²⁺ ions for Sr_{0.77-x}Na_xCa_{0.2}Al_{2-x}Si_{2+x}O₈:0.03Eu²⁺.

value	Lifetime (ns)
x=0	480.551
x=0.1	493.51
x=0.2	504.88
x=0.3	507.793
x=0.4	509.957
x=0.5	510.266
x=0.6	520.594
x=0.7	537.20

Table S5 The life times of Eu²⁺ ions for Sr_{0.97-y}Ca_yAl₂Si₂O₈:0.03Eu²⁺.

value	Lifetime (ns)
y=0	510.78
y=0.1	523.277
y=0.2	539.450
y=0.3	543.106
y=0.4	559.837
y=0.5	561.632
y=0.6	585.054
y=0.7	589.672
y=0.8	604.060
y=0.97	612.770

Table S6 The CIE chromaticity coordinates, internal quantum efficiency (IQE) and color purity (CP) of representative samples for two series.

Sr _{0.77-x} Na _x Ca _{0.2} Al _{2-x} Si _{2+x} O ₈ :0.03Eu ²⁺				Sr _{0.97-y} Ca _y Al ₂ Si ₂ O ₈ :0.03Eu ²⁺			
value	CIE (X,Y)	IQE (%)	CP(%)	value	CIE (X,Y)	IQE (%)	CP(%)
x=0	(0.1653, 0.1057)	77.02	83.5	y=0	(0.1597, 0.0998)	75.85	81.8
x=0.2	(0.1605, 0.0918)	79.35	82.9	y=0.3	(0.1600, 0.0934)	80.05	80.2
x=0.4	(0.1635, 0.0991)	80.68	80.3	y=0.5	(0.1618, 0.1047)	83.77	77.6
x=0.7	(0.1631, 0.1111)	84.02	79.6	y=0.8	(0.1627, 0.1175)	85.56	75.4
				y=0.97	(0.1637, 0.1628)	89.04	72.1