

Electronic Supplementary Information (ESI)

Broadly Color Tuning of Bi³⁺/Eu³⁺ Doped (Ba,Sr)₃Sc₄O₉ Solid Solution Compounds via Crystal Field Modulation and Energy Transfer

Peipei Dang,^{a,b,d} Sisi Liang,^{b,d} Guogang Li,^{*,c} Hongzhou Lian,^b Mengmeng Shang,^e and Jun Lin^{*,a,b,d}

^a School of Applied Physics and Materials, Wuyi University, Jiangmen, Guangdong, 529020, P. R., China

^b State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R., China
*E-mail: jlin@ciac.ac.cn

^c Engineering Research Center of Nano-Geomaterials of Ministry of Education, Faculty of Materials Science and Chemistry, China University of Geosciences, 388 Lumo Road, Wuhan 430074, P. R., China. *E-mail: ggli@cug.edu.cn

^d University of Science and Technology of China, Hefei, 230026, China

^e School of Chemistry and Chemical Engineering, Qingdao University, 308 Ningxia Road, Qingdao, 266071, P. R. China

Table S1. Bond distances between the Sr atoms and O atoms in Sr₃Sc₄O₉ host.

Sr1-O _i		Sr2-O _i		Sr3-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Sr1-O1	2.6829	Sr2-O1	2.6830	Sr3-O1	2.5030
Sr1-O1	2.6829	Sr2-O1	2.6830	Sr3-O1	2.5030
Sr1-O1	2.6829	Sr2-O1	2.6830	Sr3-O1	2.5030
Sr1-O3	3.1897	Sr2-O2	2.9719	Sr3-O1	3.1844
Sr1-O3	3.1897	Sr2-O2	2.9719	Sr3-O1	3.1844
Sr1-O3	3.1897	Sr2-O2	2.9719	Sr3-O1	3.1844
Sr1-O3	2.5787			Sr3-O2	3.3505
Sr1-O3	2.5787			Sr3-O2	3.3505
Sr1-O3	2.5787			Sr3-O2	3.3505
				Sr3-O3	3.1896
				Sr3-O3	3.1896
				Sr3-O3	3.1896
Average Sr1-O	2.8771	Average Sr2-O	2.8275	Average Sr3-O	3.0569

Table S2. Bond distances between the Sc atoms and O atoms in Sr₃Sc₄O₉ host.

Sc1-O _i		Sc2-O _i		Sc3-O _i		Sc4-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Sc1-O2	1.8851	Sc2-O1	2.0170	Sc3-O2	1.9576	Sc4-O1	2.1108
Sc1-O2	1.8851	Sc2-O1	2.0170	Sc3-O2	1.9576	Sc4-O1	2.1108
Sc1-O2	1.8851	Sc2-O1	2.0170	Sc3-O2	1.9576	Sc4-O1	2.1108
Sc1-O3	2.2452	Sc2-O2	2.3472	Sc3-O3	2.0940	Sc4-O3	2.0745
Sc1-O3	2.2452	Sc2-O2	2.3472	Sc3-O3	2.0940	Sc4-O3	2.0745
Sc1-O3	2.2452	Sc2-O2	2.3472	Sc3-O3	2.0940	Sc4-O3	2.0745
Average Sc1-O	2.0652	Average Sc2-O	2.1821	Average Sc3-O	2.0258	Average Sc4-O	2.0927

Table S3. Bond distances between the Sr atoms and O atoms in $\text{Sr}_{2.97}\text{Sc}_4\text{O}_9:0.03\text{Bi}^{3+}$ sample.

Sr1-O _i		Sr2-O _i		Sr3-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Sr1-O1	2.6775	Sr2-O1	2.6311	Sr3-O1	2.5173
Sr1-O1	2.6775	Sr2-O1	2.6311	Sr3-O1	2.5173
Sr1-O1	2.6775	Sr2-O1	2.6311	Sr3-O1	2.5173
Sr1-O3	3.1708	Sr2-O2	2.9406	Sr3-O1	3.1649
Sr1-O3	3.1708	Sr2-O2	2.9406	Sr3-O1	3.1649
Sr1-O3	3.1708	Sr2-O2	2.9406	Sr3-O1	3.1649
Sr1-O3	2.6128			Sr3-O2	3.3464
Sr1-O3	2.6128			Sr3-O2	3.3464
Sr1-O3	2.6128			Sr3-O2	3.3464
				Sr3-O3	3.1233
				Sr3-O3	3.1233
				Sr3-O3	3.1233
Average Sr1-O	2.8204	Average Sr2-O	2.7858	Average Sr3-O	3.0379

Table S4. Bond distances between the Sc atoms and O atoms in $\text{Sr}_{2.97}\text{Sc}_4\text{O}_9\text{:0.03Bi}^{3+}$ sample.

Sc1-O _i		Sc2-O _i		Sc3-O _i		Sc4-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Sc1-O2	2.0477	Sc2-O1	2.1558	Sc3-O2	2.2491	Sc4-O1	1.9631
Sc1-O2	2.0477	Sc2-O1	2.1558	Sc3-O2	2.2491	Sc4-O1	1.9631
Sc1-O2	2.0477	Sc2-O1	2.1558	Sc3-O2	2.2491	Sc4-O1	1.9631
Sc1-O3	2.1339	Sc2-O2	2.0774	Sc3-O3	1.9262	Sc4-O3	2.2570
Sc1-O3	2.1339	Sc2-O2	2.0774	Sc3-O3	1.9262	Sc4-O3	2.2570
Sc1-O3	2.1339	Sc2-O2	2.0774	Sc3-O3	1.9262	Sc4-O3	2.2570
Average Sc1-O	2.0908	Average Sc2-O	2.1166	Average Sc3-O	2.0877	Average Sc4-O	2.1101

Table S5. Bond distances between the Ba/Sr atoms and O atoms in $\text{Sr}_{1.47}\text{Ba}_{1.5}\text{Sc}_4\text{O}_9\text{:0.03Bi}^{3+}$ sample.

Ba1/Sr1-O _i		Ba2/Sr2-O _i		Ba3/Sr3-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Ba1/Sr1-O1	2.7028	Ba2/Sr2-O1	2.7780	Ba3/Sr3-O1	2.5408
Ba1/Sr1-O1	2.7028	Ba2/Sr2-O1	2.7780	Ba3/Sr3-O1	2.5408
Ba1/Sr1-O1	2.7028	Ba2/Sr2-O1	2.7780	Ba3/Sr3-O1	2.5408
Ba1/Sr1-O3	3.1984	Ba2/Sr2-O2	2.3544	Ba3/Sr3-O1	3.1939
Ba1/Sr1-O3	3.1984	Ba2/Sr2-O2	2.3544	Ba3/Sr3-O1	3.1939
Ba1/Sr1-O3	3.1984	Ba2/Sr2-O2	2.3544	Ba3/Sr3-O1	3.1939
Ba1/Sr1-O3	2.6351			Ba3/Sr3-O2	3.4810
Ba1/Sr1-O3	2.6351			Ba3/Sr3-O2	3.4810
Ba1/Sr1-O3	2.6351			Ba3/Sr3-O2	3.4810
				Ba3/Sr3-O3	3.2617
				Ba3/Sr3-O3	3.2617
				Ba3/Sr3-O3	3.2617
Average Ba1/Sr1-O	2.8454	Average Ba2/Sr2-O	2.5662	Average Ba3/Sr3-O	3.1194

Table S6. Bond distances between the Ba atoms and O atoms in Ba_{2.97}Sc₄O₉:0.03Bi³⁺ sample.

Ba1-O _i		Ba2-O _i		Ba3-O _i	
Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Ba1-O1	2.7807	Ba2-O1	2.8067	Ba3-O1	2.5725
Ba1-O1	2.7807	Ba2-O1	2.8067	Ba3-O1	2.5725
Ba1-O1	2.7807	Ba2-O1	2.8067	Ba3-O1	2.5725
Ba1-O3	3.2264	Ba2-O2	2.6205	Ba3-O1	3.2333
Ba1-O3	3.2264	Ba2-O2	2.6205	Ba3-O1	3.2333
Ba1-O3	3.2264	Ba2-O2	2.6205	Ba3-O1	3.2333
Ba1-O3	2.6540			Ba3-O2	3.2657
Ba1-O3	2.6540			Ba3-O2	3.2657
Ba1-O3	2.6540			Ba3-O2	3.2657
				Ba3-O3	3.3157
				Ba3-O3	3.3157
				Ba3-O3	3.3157
Average Ba1-O	2.8870	Average Ba2-O	2.7136	Average Ba3-O	3.0968

Table S7. The emission wavelengths and FWHMs of $\text{Sr}_{2.97}\text{Sc}_4\text{O}_9:0.03\text{Bi}^{3+}$ sample excited at different sites.

$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	EM1/nm	FWHM/nm	EM2/nm	FWHM /nm
300	497	551.9	120.15	488.51	82.67
310	512	556.48	119.88	496.82	84.71
315	517	557.60	119.75	499.95	84.80
320	523	560.76	118.79	504.71	85.54
325	529	563.00	118.53	508.28	86.28
330	534	565.30	118.06	512.90	87.67
335	536	568.15	117.47	516.78	89.08
340	538	572.19	112.85	517.94	87.96
342	540	571.04	117.82	517.50	86.10

Table S8. The internal quantum yields (IQYs) of BSSO:0.03Bi³⁺ ($x = 0-3.0$) and SSO:0.03Bi³⁺,_zEu³⁺ ($z = 0-0.30$) under 330 nm wavelength excitation.

Samples (BSSO)	IQYs	Samples (SSO)	IQYs
$x = 0$	10.3%	$z = 0$	32.2%
$x = 0.5$	9.50%	$z = 0.03$	29.3%
$x = 1.0$	18.1%	$z = 0.06$	34.9%
$x = 1.5$	22.0%	$z = 0.12$	28.7%
$x = 2.0$	22.2%	$z = 0.15$	23.1%
$x = 2.5$	34.1%	$z = 0.20$	34.1%
$x = 3.0$	32.2%	$z = 0.30$	33.9%

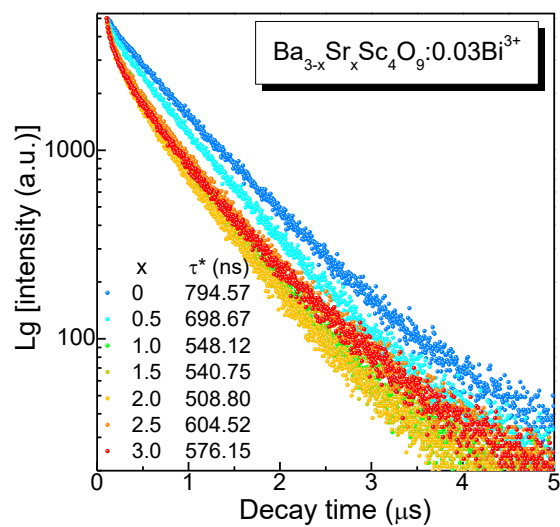


Fig. S1 The luminescence decay curves of $\text{Ba}_{3-x}\text{Sr}_x\text{Sc}_4\text{O}_9:0.03\text{Bi}^{3+}$ ($x = 0-3.0$) monitored at different emission wavelength (464-526 nm), with excitation wavelength of 375 nm.

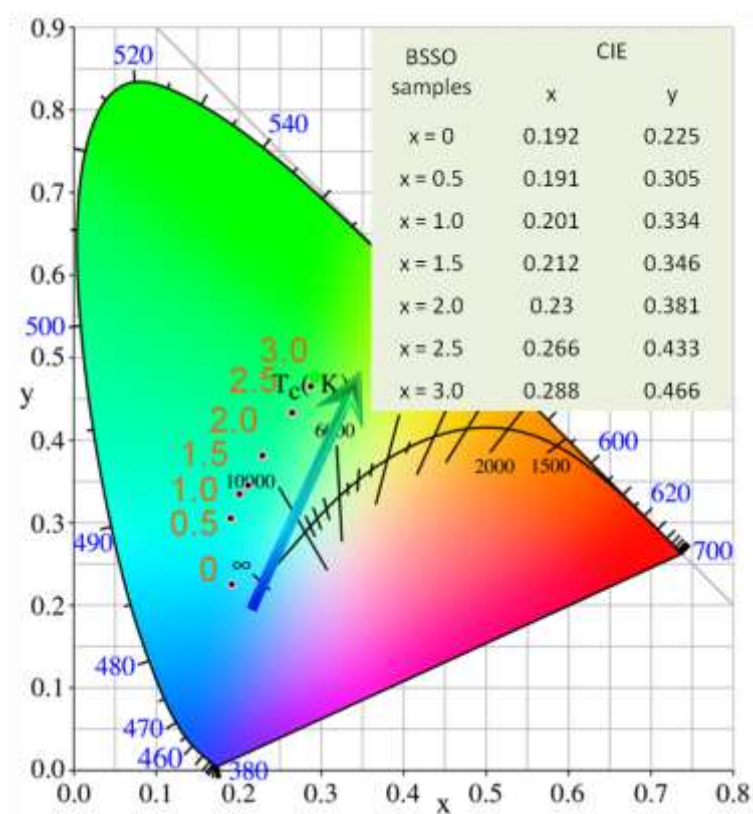


Fig. S2 The corresponding CIE chromaticity coordinates diagram of BSSO:0.03Bi³⁺ samples under 330 nm wavelength excitation, with different x values.

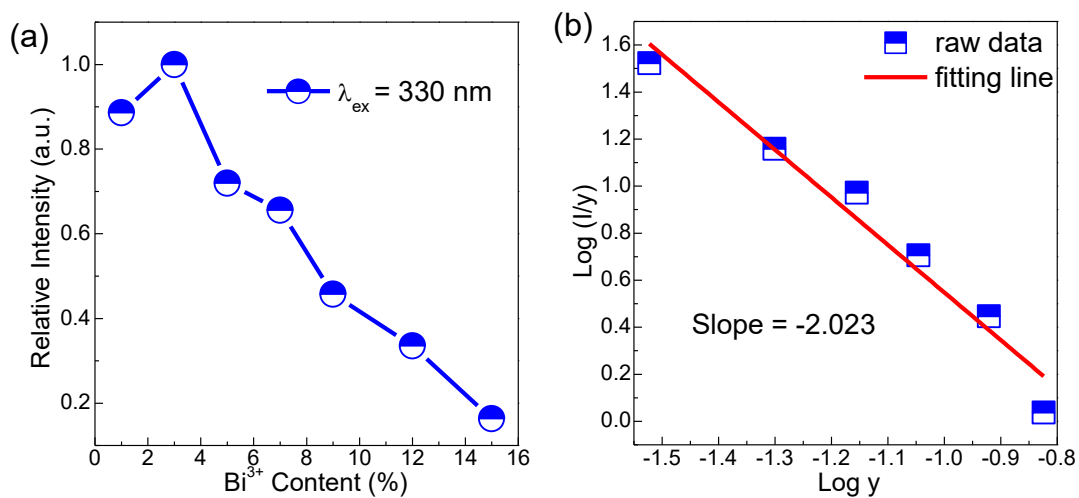


Fig. S3 (a) Variation of Bi³⁺ emission intensity as a function of Bi³⁺ content (y) in SSO:yBi³⁺ samples. (b) The best linear fitting relationship between $\log(I/y)$ and $\log y$ of Bi³⁺ ions.

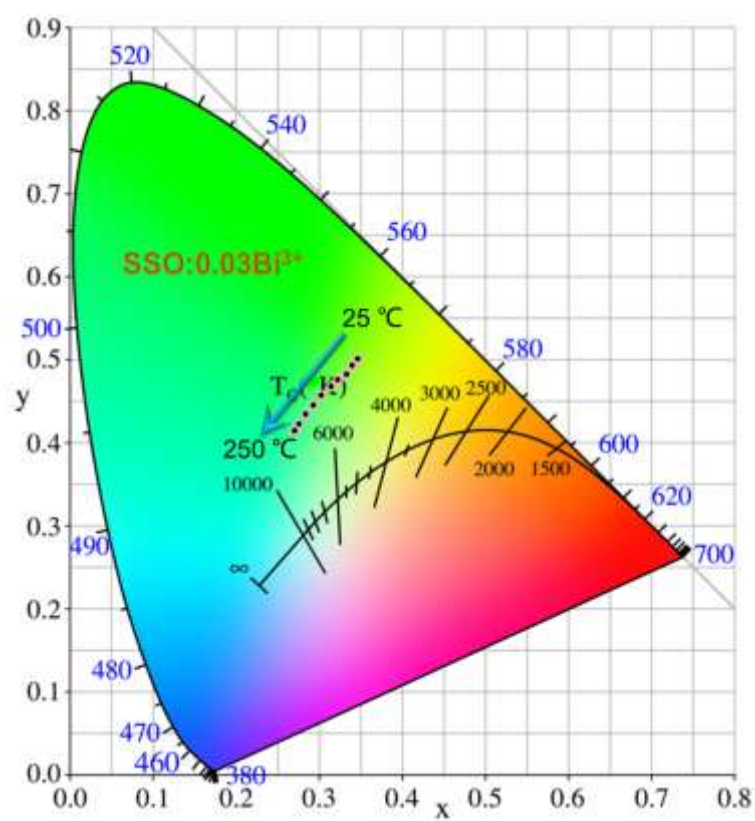


Fig.S4 The CIE chromaticity coordinates diagram of SSO:0.03Bi³⁺ sample under 330 nm wavelength excitation at various temperatures (25-250 °C).

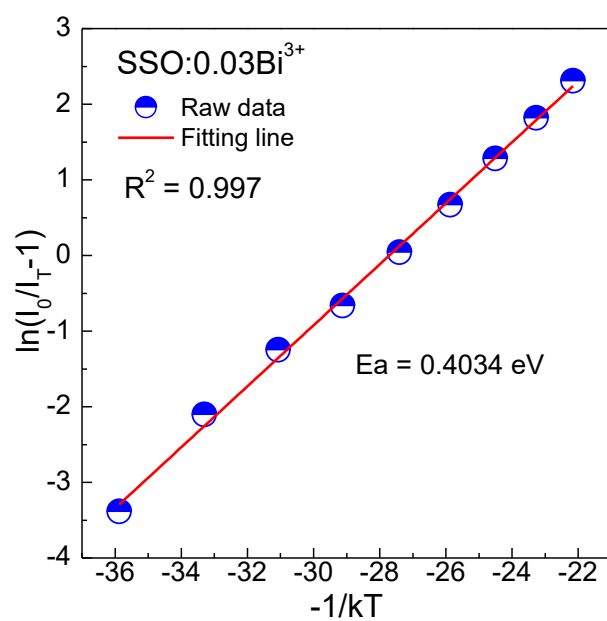


Fig. S5 The Linear relationship of the $\ln(I_0/I_T - 1)$ versus $(-1/kT)$ activation energy graph for thermal quenching of the SSO:0.03Bi³⁺ sample.