Supporting Information

Interplay between local environments and photoluminescence of Eu^{2+} in $Ba_2Zr_2Si_3O_{12}$: blue shift emission, optimal bond valence and luminescence mechanisms

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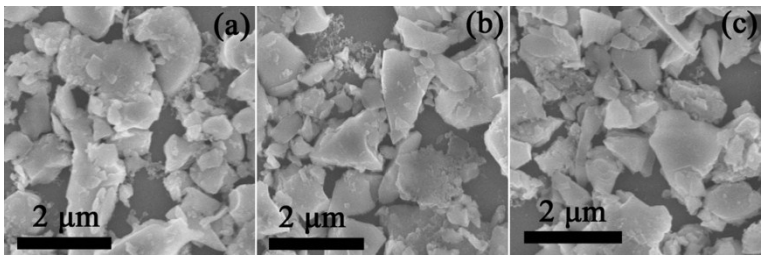

Fig. S1 The SEM images of (a) BZSO: 0.03Eu^{2+}, (b) BZSO: 0.03Eu^{2+}, 0.10Ca^{2+}, (c) BZSO: 0.03Eu^{2+}, 5 0.10Sr^{2+}.

Table S1. Crystallographic data of $Ba_2Zr_2Si_3O_{12}$: $0.03Eu^{2+}$, as determined by the Rietveld refinement of power XRD data at room temperature.

atom	site	*x*	*y*	*z*	Occupancy
Ba1	4*a*	0.568	0.568	0.568	0.985
Ba2	4*a*	0.797	0.797	0.797	0.985
Zr1	4*a*	0.084	0.084	0.084	1.00
Zr2	4*a*	0.35	0.35	0.35	1.00
Si1	12*b*	0.033	0.268	0.375	1.00
O1	12*b*	0.012	0.196	0.246	1.00
O2	12*b*	0.173	0.258	0.427	1.00
O3	12*b*	0.021	0.057	0.713	1.00
O4	12*b*	0.002	0.412	0.349	1.00
Eu1	4*a*	0.568	0.568	0.568	0.015
Eu2	4*a*	0.797	0.797	0.797	0.015

Space group: $P2_13$ (No. 198), $Z = 4$, $a = b = c = 10.24278$ Å, $V = 1074.62$ Å^3, $\alpha = \beta = \gamma = 90°$, $R_p = 6.05\%$, $R_{wp} = 7.76\%$.

Table S2. Crystallographic data and reliability factor of BZSO: 0.03Eu^{2+}, *m*Ca^{2+} (*m* = 0.03−0.10) and BZSO: 0.03Eu^{2+}, *n*Sr^{2+} (*n* = 0.03−0.10) materials.

BZSO: 0.03Eu^{2+}, *m*Ca^{2+}					
m	*m* = 0.03	*m* = 0.05	*m* = 0.06	*m* = 0.08	*m* = 0.10
a = *b* = *c*	10.23848	10.23687	10.23677	10.23619	10.23066
cell volume	1073.26	1072.76	1072.72	1072.54	1070.80
R_p	6.46%	6.18%	6.62%	6.5%	6.56%
R_{wp}	8.16%	8.18%	8.94%	8.41%	8.71%
BZSO: 0.03Eu^{2+}, *n*Sr^{2+}					
n	*n* = 0.03	*n* = 0.05	*n* = 0.06	*n* = 0.08	*n* = 0.10
a = *b* = *c*	10.23942	10.23879	10.23843	10.23664	10.23072
cell volume	1073.56	1073.36	1073.24	1072.68	1070.82
R_p	6.27%	6.51%	6.36%	6.08%	6.19%
R_{wp}	8.19%	8.61%	8.5%	7.73%	8%

Table S3. Excitation, emission, centre of gravity, Stokes shift and crystal filed splitting and the CIE coordinates of of BZSO: 0.03Eu^{2+}, *m*Ca^{2+}/*n*Sr^{2+}.

Samples	λ_{em} nm	Stokes shift cm^{-1}	Centre of gravity cm^{-1}	Crystal field splitting cm^{-1}	CIE (*x, y*)
BZSO:0.03Eu^{2+}	501	5292	30832	9737	(0.191, 0.412)
BZSO:0.03Eu^{2+}, *m*Ca^{2+}					
0.01	497	5132	30991	9382	(0.181, 0.347)
0.03	495	5050	31880	9276	(0.175, 0.329)
0.05	490	4844	32017	9488	(0.168, 0.280)
0.06	485	4633	32017	10139	(0.170, 0.277)
0.08	478	4332	32573	11888	(0.167, 0.270)
0.10	472	4066	32644	12655	(0.165, 0.243)
BZSO:0.03Eu^{2+}, *n*Sr^{2+}					
0.01	497	5131	30959	9307	(0.174, 0.363)
0.03	496	5091	31779	9140	(0.176, 0.323)
0.05	492	4927	32085	9412	(0.166, 0.305)
0.06	488	4760	32188	9840	(0.171, 0.283)
0.08	483	4548	32223	9397	(0.170, 0.279)
0.10	480	4419	32327	9380	(0.163, 0.274)

Table S4. The decay life times of Eu^{2+} in BZSO: $0.03Eu^{2+}$, mCa^{2+} (m = 0.03−0.10) and BZSO: $0.03Eu^{2+}$, nSr^{2+} (n = 0.03−0.10) materials.

BZSO: $0.03Eu^{2+}$, mCa^{2+}					
m	m = 0.03	m = 0.05	m = 0.06	m = 0.08	m = 0.10
τ (μs)	0.894	0.765	0.797	1.149	1.156
BZSO: $0.03Eu^{2+}$, nSr^{2+}					
n	n = 0.03	n = 0.05	n = 0.06	n = 0.08	n = 0.10
τ (μs)	0.908	0.853	0.871	1.202	1.337

5