Supporting Information

Tuning crystal structure and luminescence of Eu^{2+}-activated $LiSr_{1-x}Ba_xPO_4$ solid solution for white light-emitting diodes

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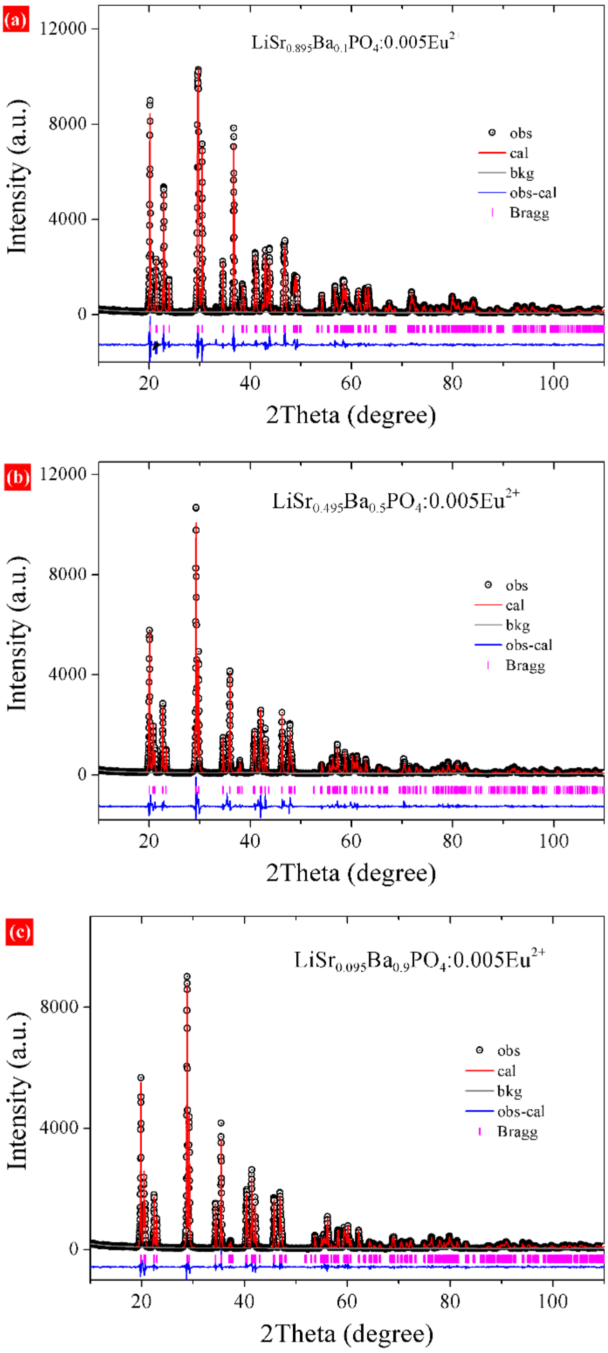

Figure S1. Rietveld refinement of $LiSr_{0.995-x}Ba_xPO_4{:}0.005Eu^{2+}$ synthesized at 1200 °C. (a) $x = 0.1$, (b) $x = 0.5$, (c) $x = 0.9$.

Table S1. Refinement Results and cell parameters for $LiSr_{0.995-x}Ba_xPO_4$:0.005Eu^{2+}

	x = 0 (1100 °C)	x = 0 (1200 °C)	0.1	0.3	0.5	0.7	0.9	0.995
Crystal	monoclinic							trigonal
S. G.*	C1c1							P31c
a/Å	5.1829(1)	5.1839(1)	5.1886(1)	5.1932(1)	5.1918(1)	5.2052(1)	5.2209(1)	5.1298(1)
b/Å	8.2776(1)	8.2788(2)	8.3219(1)	8.4411(1)	8.5644(2)	8.6319(2)	8.6895(1)	--
c/Å	8.2233(1)	8.2212(2)	8.2617(1)	8.3444(1)	8.4272(2)	8.5063(1)	8.5912(1)	8.6644(1)
V/Å^3	352.77(1)	352.82(1)	356.73(1)	365.78(1)	374.71(1)	382.20(1)	389.75(1)	197.46(1)
β/°	90.36	90.35	90.34	90.18	89.97	90.04	89.89	90
Z	4	4	4	4	4	4	4	2
R_{wp}	9.97%	15.49%	9.60%	10.01%	13.29%	12.63%	9.02%	12.78%
R_p	6.26%	9.93%	6.36%	6.85%	9.21%	8.89%	6.23%	9.20%
χ^2	3.043	8.435**	2.792	2.416	3.606	2.687	1.377	2.411

*space group,

**There is an obvious impurity for x = 0 (1200 °C) as indicated in our previous work.[1] Therefore, a higher χ^2 value is obtained.

[1] Liao, S.; Li, Y.; Zhang, Y.; Tan, Z.; Fu, X.; Qiu, Z.; Zhang, J., Highly thermal stable phosphor $LiSrPO_4$:Eu^{2+} with a new crystal structure. *Applied Materials Today* **2020**, *21*, 100792.

Table S2. Atomic parameters of $LiSr_{0.995}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.995	0.13458	0.00771	-0.15128	0.0074
Eu	4a	0.005	0.13458	0.00771	-0.15128	0.0074
P	4a	1	0.13192	0.31069	0.57779	0.0035
O1	4a	1	-0.16482	0.20133	0.21813	0.0137
O2	4a	1	-0.03622	0.15405	0.58223	0.0101
O3	4a	1	0.45663	-0.04824	0.60296	0.0064
O4	4a	1	-0.25397	0.80594	0.40881	0.0096
Li	4a	1	0.08191	0.38585	0.15789	0.0137

Table S3. Atomic parameters of $LiSr_{0.895}Ba_{0.1}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.895	0.09480	0.00792	-0.24102	0.0121
Ba	4a	0.1	0.09480	0.00792	-0.24102	0.0121
Eu	4a	0.005	0.09480	0.00792	-0.24102	0.0121
P	4a	1	0.07929	0.31176	0.49035	0.0064
O1	4a	1	-0.20720	0.19576	0.12438	0.0125
O2	4a	1	-0.07595	0.15720	0.49669	0.0099
O3	4a	1	0.40921	-0.04505	0.51336	0.0006
O4	4a	1	-0.29438	0.81797	0.31876	0.0007
Li	4a	1	0.07424	0.37463	0.07013	0.0051

Table S4. Atomic parameters of $LiSr_{0.695}Ba_{0.3}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.695	0.09237	-0.00782	-0.24764	0.0150
Ba	4a	0.3	0.09237	-0.00782	-0.24764	0.0150
Eu	4a	0.005	0.09237	-0.00782	-0.24764	0.0150
P	4a	1	0.09232	0.31989	0.53027	0.0055
O1	4a	1	-0.32309	0.18887	0.19764	0.0801
O2	4a	1	-0.07909	0.16672	0.50640	0.0121
O3	4a	1	0.41628	-0.05247	0.50193	0.0211
O4	4a	1	-0.16883	0.80265	0.39912	0.0435
Li	4a	1	-0.04435	0.38244	-0.05344	0.0231

Table S5. Atomic parameters of $LiSr_{0.495}Ba_{0.5}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.495	0.08980	-0.00688	-0.26275	0.0153
Ba	4a	0.5	0.08980	-0.00688	-0.26275	0.0153
Eu	4a	0.005	0.08980	-0.00688	-0.26275	0.0153
P	4a	1	0.08405	0.32096	0.51916	0.0115
O1	4a	1	-0.32367	0.18068	0.19251	0.0241
O2	4a	1	-0.07443	0.17345	0.47942	0.0057
O3	4a	1	0.41733	-0.03951	0.50373	0.0112
O4	4a	1	-0.17200	0.81878	0.40850	0.0169
Li	4a	1	0.14386	0.36480	-0.08656	0.0192

Table S6. Atomic parameters of $LiSr_{0.295}Ba_{0.7}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.295	0.07613	-0.00784	-0.26701	0.0127
Ba	4a	0.7	0.07613	-0.00784	-0.26701	0.0127
Eu	4a	0.005	0.07613	-0.00784	-0.26701	0.0127
P	4a	1	0.07988	0.32443	0.51390	0.0114
O1	4a	1	-0.34975	0.17413	0.18824	0.0129
O2	4a	1	-0.08824	0.17795	0.47031	0.0035
O3	4a	1	0.41594	-0.03907	0.48423	0.0109
O4	4a	1	-0.18197	0.82123	0.41150	0.0205
Li	4a	1	0.13918	0.35731	-0.09318	0.0039

Table S7. Atomic parameters of $LiSr_{0.095}Ba_{0.9}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Sr	4a	0.095	0.06931	-0.00730	-0.26705	0.0110
Ba	4a	0.9	0.06931	-0.00730	-0.26705	0.0110
Eu	4a	0.005	0.06931	-0.00730	-0.26705	0.0110
P	4a	1	0.08207	0.32917	0.52208	0.0028
O1	4a	1	-0.37681	0.17653	0.20869	0.0623
O2	4a	1	-0.10093	0.17072	0.50041	0.0269
O3	4a	1	0.40921	-0.03654	0.47981	0.0069
O4	4a	1	-0.18998	0.82392	0.51741	0.0257
Li	4a	1	0.03941	0.35087	-0.09316	0.0569

Table S8. Atomic parameters of $LiBa_{0.995}PO_4$:0.005Eu^{2+}

Atom	**Wyckoff**	**S.O.F.**	***x/a***	***y/b***	***z/c***	**U_{iso}/[Å^2]**
Ba	2a	0.995	0	0	0.02922	0.0089
Eu	2a	0.005	0	0	0.02922	0.0089
P	2b	1	2/3	1/3	0.82194	0.0027
O1	2b	1	2/3	1/3	0.99106	0.0415
O2	6c	1	0.38980	0.05364	0.76357	0.0068
Li	2b	1	2/3	1/3	0.18632	0.3027

Table S9. Sr/Ba/Eu-O and P-O distances (*d*) of selected samples from the refinement results.

sample (*x*)	Sr/Ba/Eu-O	*d* (Å)	P-O	*d* (Å)
$LiSr_{0.995}PO_4$:0.005Eu^{2+}, (x = 0)	O1	2.5566	O1	1.5609
	O1	2.8373	O2	1.5631
	O2	2.6510	O3	1.4949
	O2	2.5067	O4	1.5138
	O3	2.6693		
	O3	2.6881		
	O4	2.5872		
	O4	2.7050		
	O4	3.5570		
$LiSr_{0.695}Ba_{0.3}PO_4$:0.005Eu^{2+}, (x = 0.3)	O1	2.6820	O1	1.4645
	O1	2.7660	O2	1.5820
	O1	3.4304	O3	1.4322
	O2	2.6766	O4	1.6632
	O2	2.6641		
	O3	2.7130		
	O3	2.7209		
	O4	2.5198		
	O4	3.0367		
$LiSr_{0.295}Ba_{0.7}PO_4$:0.005Eu^{2+}, (x = 0.7)	O1	2.6681	O1	1.5273
	O1	2.9311	O2	1.5817
	O1	3.3373	O3	1.4764
	O2	2.8800	O4	1.5158
	O2	2.6392		
	O3	2.7719		
	O3	2.8026		
	O4	3.3476		
	O4	2.5900		
$LiBa_{0.995}PO_4$:0.005Eu^{2+}, (x = 0.995)	O2	2.9702	O1	1.4654
	O2	2.9702	O2	1.5145
	O2	2.9702	O2	1.5143
	O1	2.9798	O2	1.5148
	O1	2.9803		
	O1	2.9803		
	O2	2.7653		
	O2	2.7653		
	O2	2.7653		

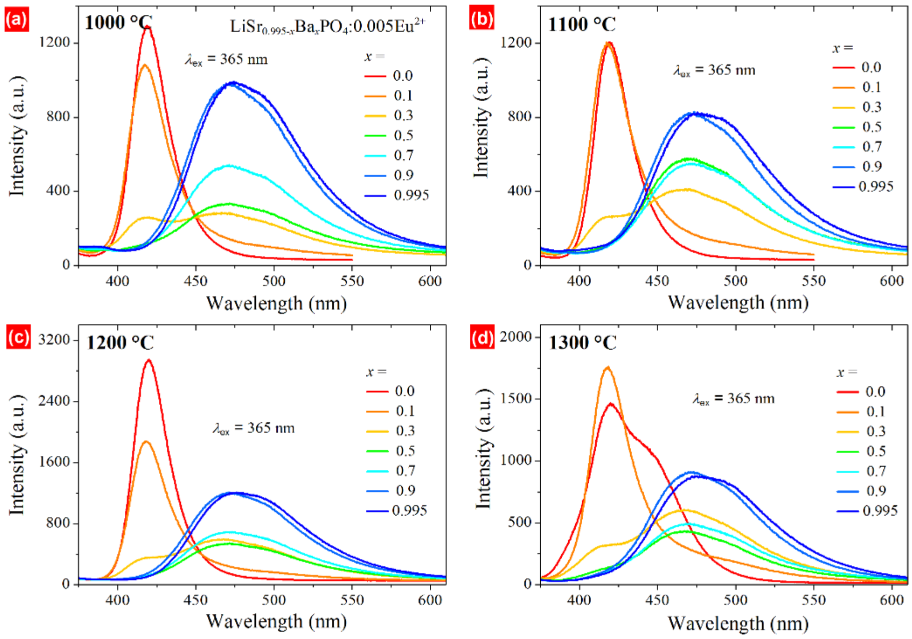

Figure S2. Comparison among PL spectra of LiSr$_{0.995-x}$Ba$_x$PO$_4$:0.005Eu^{2+} obtained at (a) 1000, (b) 1100, (c) 1200, and (d) 1300 °C.

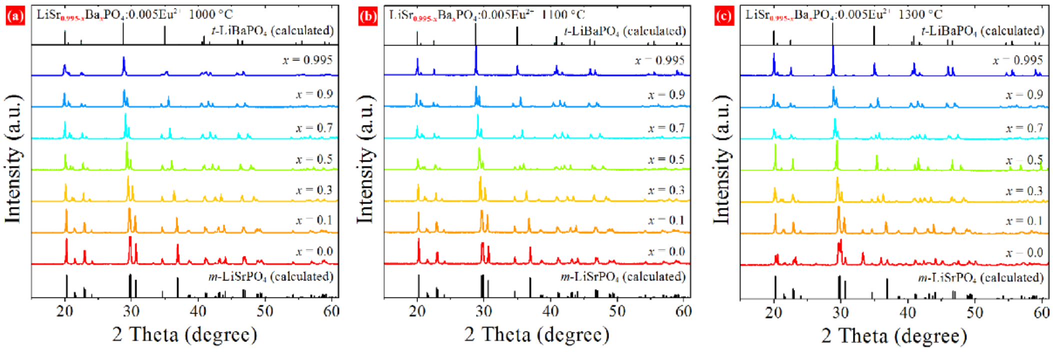

Figure S3. XRD patterns of LiSr$_{0.995-x}$Ba$_x$PO$_4$:0.005Eu^{2+} obtained at (a) 1000, (b) 1100, (c) 1300 °C.

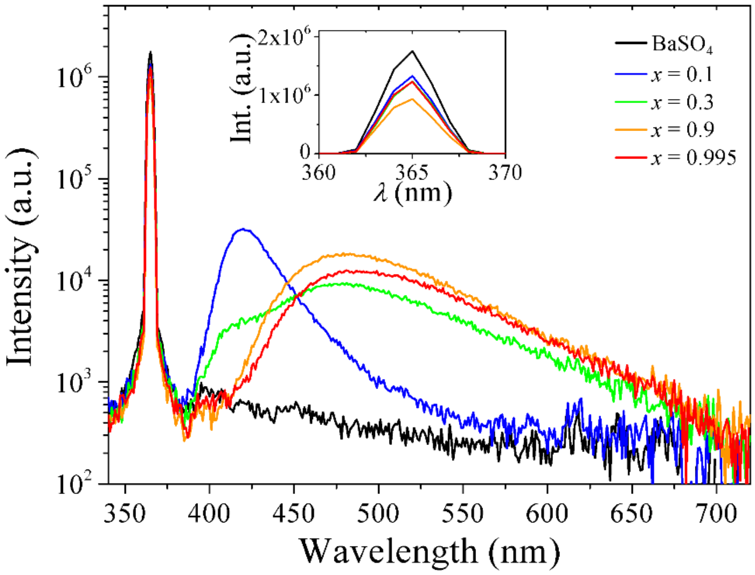

Figure S4. Spectra for the measurement of quantum efficiency.

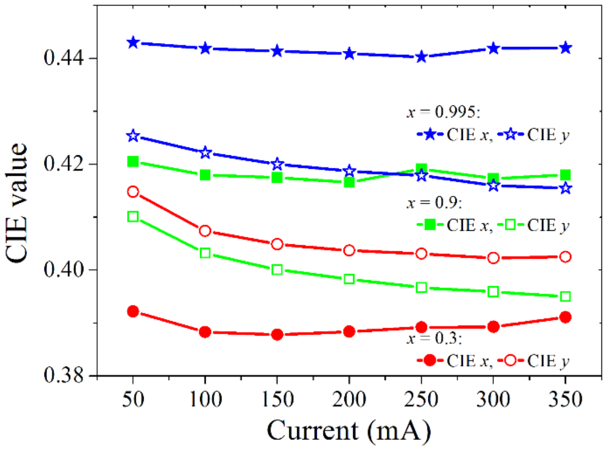

Figure S5. CIE coordinate values versus driving current.