

Supplementary Information

Realizing cool and warm white-LEDs based on color controllable (Sr, Ba)₂Al₃O₆F: Eu²⁺ phosphors obtained via a microwave-assisted diffusion method

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Table S1: The table shows the lattice parameter of the following refined samples.

Lattice parameters	Sr ₂ Al ₃ O ₆ F	Sr _{1.95} Al ₃ O ₆ F: 0.05Eu ²⁺	Sr _{1.85} Ba _{0.1} Al ₃ O ₆ F: 0.05Eu ²⁺
a [Å]	17.32375	17.52476	17.831
b [Å]	17.32375	17.52476	17.831
c [Å]	7.00017	7.15817	7.224626
V[Å ³]	1819.378	1903.867	1989.012
Rp (%)	7.2	6.8	5.6
Rwp (%)	10.3	9.2	7.3

Table S2: The table shows the atomic coordinates, fractional occupancies and isotropic displacement parameters of the following compounds.

Sr₂Al₃O₆F						
Atom	Site	x	y	z	Occ.	B_{iso}
Sr1	18f	0.22320	0.41486	0.07597	1.0	2.243
Sr2	6c	0.00000	0.00000	0.27710	1.0	2.63
Al1	18f	0.59279	0.45660	0.29840	1.0	1.846
Al2	18f	0.64325	0.05015	0.10267	1.0	1.819
O1	18f	0.59430	0.54030	0.44580	1.0	1.57
O2	18f	0.14001	0.11132	0.11725	1.0	2.59
O3	18f	0.55819	0.07728	0.11751	1.0	2.16
O4	18f	0.60087	-0.05778	0.19406	1.0	1.98
F1	18f	0.34113	0.56813	0.17990	0.667	7.6

Sr_{1.95}Al₃O₆F: 0.05Eu²⁺						
Atom	Site	x	y	z	Occ.	B_{iso}
Sr1	18f	0.22240	0.43487	0.43487	0.995	2.235
Eu1	18f	0.22240	0.43487	0.43487	0.005	2.235
Sr2	6c	0.00000	0.00000	0.26910	0.985	2.710
Eu2	6c	0.00000	0.00000	0.26910	0.015	2.710
Al1	18f	0.59863	0.48560	0.29840	1.0	1.846
Al2	18f	0.64325	0.05015	0.10267	1.0	1.829
O1	18f	0.59430	0.57030	0.44580	1.0	1.570
O2	18f	0.14001	0.12150	0.11689	1.0	2.580
O3	18f	0.55819	0.07728	0.11751	1.0	2.360
O4	18f	0.59087	-0.05678	0.19806	1.0	1.890
F1	18f	0.34113	0.56813	0.17990	0.667	7.650

Sr_{1.85}Ba_{0.1}Al₃O₆F: 0.05Eu²⁺						
Atom	Site	x	y	z	Occ.	B_{iso}
Sr1	18f	0.22515	0.41278	0.07182	0.950	0.021
Eu1	18f	0.24195	0.42515	0.09977	0.050	-0.61
Sr2	6c	0.00000	0.00000	0.26413	0.850	-0.089
Eu2	6c	0.00000	0.00000	0.26288	0.050	-0.5
Ba2	6c	0.00000	0.00000	0.26360	0.100	0.2
Al1	18f	0.59318	0.45486	0.31397	1.0	0.018
Al2	18f	0.64215	0.04782	0.13585	1.0	-0.042
O1	18f	0.59536	0.53120	0.43280	1.0	-0.271
O2	18f	0.12773	0.10096	0.10625	1.0	-0.65
O3	18f	0.55500	0.06859	0.10211	1.0	-0.59
O4	18f	0.61347	-0.05636	0.21042	1.0	-1.71
F1	18f	0.415	0.541	0.098	0.667	0.025

Table S3: The bonds and corresponding bond lengths that exist between the elements in the following samples.

Sr₂Al₃O₆F		Sr_{1.95}Al₃O₆F: 0.05Eu²⁺		Sr_{1.85}Ba_{0.1}Al₃O₆F: 0.05Eu²⁺	
Bond type	Bond length [Å]	Bond type	Bond length [Å]	Bond type	Bond length [Å]
Sr1-O1 × 2	2.572 (2)	Sr1-O1 × 2	2.785 (2)	Sr1-O1 × 2	2.659 (2)
Sr1-O2 × 1	2.681 (1)	Sr1-O2 × 1	2.64 (1)	Sr1-O3 × 2	2.643 (2)
Sr1-O3 × 2	2.637 (2)	Sr1-O3 × 2	2.825 (2)	Sr1-O4 × 2	2.636 (2)
Sr1-O4 × 2	2.465 (2)	Sr1-O4 × 2	2.50 (2)	Sr1-F × 2	2.280 (2)
Sr1-F1 × 2	2.501 (2)	Sr1-F1 × 2	2.255 (2)	Sr1-Eu1 × 1	3.852 (1)
Sr2-O2 × 3	2.485 (3)	Sr2-O2 × 3	2.55 (3)	Sr1-Ba2 × 1	4.065 (1)
Sr2-F1 × 6	2.367 (6)	Sr2-F1 × 6	2.445 (2)	Sr1-Al1 × 1	3.288 (1)
Al1-O1 × 1	1.769 (1)	Al1-O1 × 1	1.853 (1)	Sr1-Al2 × 1	3.264 (1)
Al1-O2 × 2	1.765 (2)	Al1-O2 × 2	1.74 (1)	Sr2-Sr2 × 1	3.611 (1)
Al1-O3 × 1	1.724 (1)	Al1-O3 × 1	1.772 (1)	Sr2-Eu2 × 1	3.416 (1)
Al2-O1 × 1	1.729 (1)	Al1-O3 × 1	1.772 (1)	Sr2-Ba2 × 1	3.611 (1)
Al2-O3 × 1	1.759 (1)	Al2-O1 × 1	1.682 (1)	Sr2-O2 × 3	2.372 (3)
Al2-O4 × 2	1.753 (2)	Al2-O3 × 1	1.780 (1)	Al1-O1 × 1	1.593 (1)
		Al2-O4 × 1	1.761 (1)	Al1-O2 × 2	1.801 (2)
		Eu1-O1 × 2	2.785 (2)	Al1-O3 × 1	2.034 (1)
		Eu1-O3 × 1	2.92 (1)	Al2-O1 × 1	1.786 (1)
		Eu1-O4 × 3	2.64 (3)	Al2-O3 × 1	1.785 (1)
		Eu2-O2 × 1	2.55(1)	Al2-O4 × 2	1.823 (2)
		Eu2-F1 × 2	2.445 (2)	Eu1-O3 × 2	2.627 (2)
				Eu1-O4 × 1	2.161 (1)
				Eu1-F × 2	2.085 (2)
				Eu2-Eu2 × 2	3.611 (2)
				Eu2-Eu2 × 1	3.425 (1)
				Eu2-Ba2 × 1	3.420 (1)
				Eu2-O2 × 3	2.368 (3)
				Ba2-Sr1 × 3	4.065 (3)
				Ba2-Eu1 × 2	3.960 (2)
				Ba2-Sr2 × 2	3.611 (2)
				Ba2-Eu2 × 2	3.611 (2)
				Ba2-Ba2 × 2	3.612 (2)
				Ba2-O2 × 2	2.370 (2)