Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Achieving Efficient Violet-light-excited Blue Phosphors by Nitridation for Violet-chip-based Full-spectrum Lighting

Chao Dou, Fangyi Zhao, Shengqiang Liu, Zhen Song, and Quanlin Liu*

The Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Sciences and Engineering, University of Science and Technology Beijing, Beijing 100083, China. E-mail: qlliu@ustb.edu.cn

Table S1. The atomic coordinates and occupancy of BAO based on ICSD No. 79360

Atoms	Wyckoff Position	x	y	z	Occ
Ba1	2d	0.3333	0.6667	0.7500	0.771(7)
Ba2	4f	0.6667	0.3333	0.462(4)	0.043(4)
Al1	12k	0.1662(4)	0.3324(8)	0.8956(2)	0.894(7)
Al2	4f	0.3333	0.6667	0.0237(4)	0.957(4)
Al3	4f	0.3333	0.6667	0.1758(3)	1.000
Al4	2a	0.0000	0.0000	0.0000	1.000
Al5	12k	0.839(1)	0.678(3)	0.1757(7)	0.106(7)
O1	12k	0.1579(6)	0.3158(12)	0.0494(3)	1.000
O2	12k	0.5025(6)	0.005(1)	0.1466(4)	1.000
O3	4f	0.3333	0.6667	-0.053(1)	0.957(4)
O4	4e	0.0000	0.0000	0.1451(7)	1.000
O5	2c	0.3333	0.6667	0.2500	1.000
O6	6h	0.893(6)	0.786(11)	0.2500	0.106(7)

Table S2. Ba-O bond lengths based on ICSD No. 79360.

Atom 1	Atom 2	Count	Distance (Å)
Ba1	O2	4	2.841(8)
		2	2.841(9)
	O6	1	2.19(7)
		2	2.19(3)
Ba2	O1	3	2.62(7)
		6	2.810(10)
	O2	3	2.94(8)

Table S3. The refined atomic coordinates and occupancy of $BAON_{1.0}$:Eu

Atoms	Wyckoff Position	x	y	z	Occ
Ba1	2d	0.3333	0.6667	0.7500	0.751(7)
Ba2	4f	0.6667	0.3333	0.4181(2)	0.003(1)
Al1	12k	0.1663(3)	0.3326(5)	0.8951(8)	0.983(7)
Al2	4f	0.3333	0.6667	0.0238(2)	0.951(10)
Al3	4f	0.3333	0.6667	0.1754(1)	1.000
Al4	2a	0.0000	0.0000	0.0000	1.000
Al5	12k	0.8163(10)	0.6311(2)	0.1304(5)	0.172(4)
O1	12k	0.1634(4)	0.3268(5)	0.0501(2)	1.000
O2	12k	0.5024(3)	0.0039(1)	0.1487(1)	1.000
O3	4f	0.3333	0.6667	-0.0541 (3)	0.832(4)
O4	4e	0.0000	0.0000	0.1445(4)	1.000
O5	2c	0.3333	0.6667	0.2500	1.000
O6	6h	0.9342(5)	0.8673(12)	0.2500	0.264(1)
Eu1	2d	0.3333	0.6667	0.7500	0.083(2)
Eu2	4f	0.6667	0.3333	0.4181(2)	0.044(1)

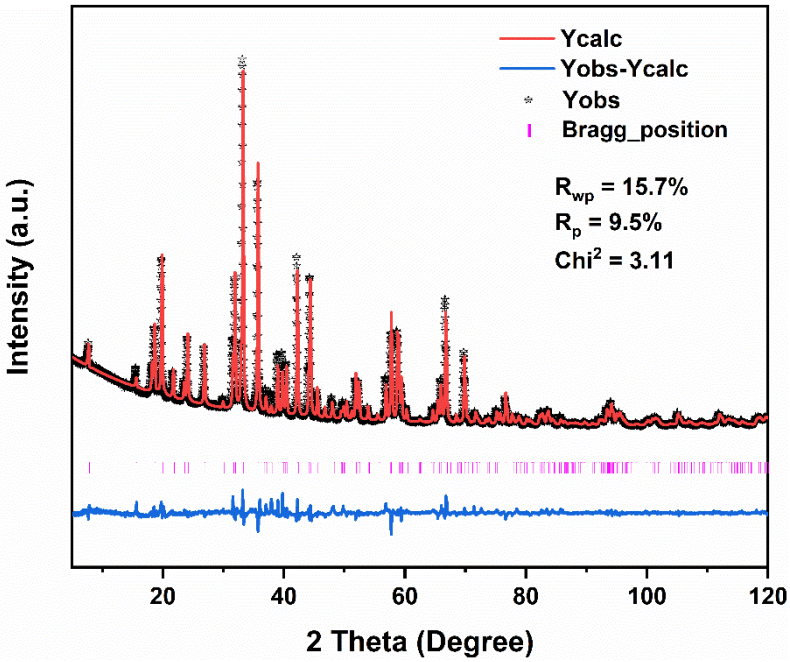

Figure S1. Rietveld refinement of the powder XRD profile of $BAON_{1.0}$:Eu.

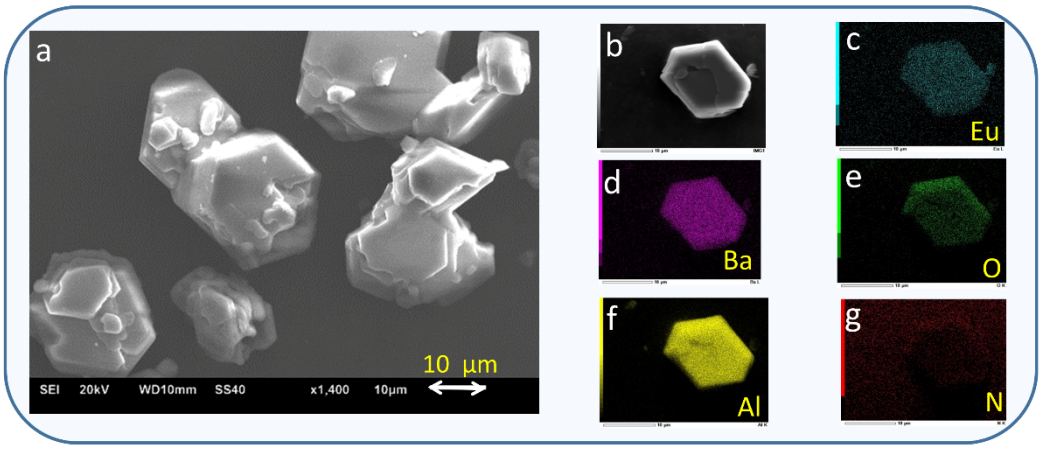

Figure S2. SEM image of $BAON_{1.0}$:Eu as well as EDS elemental mapping.

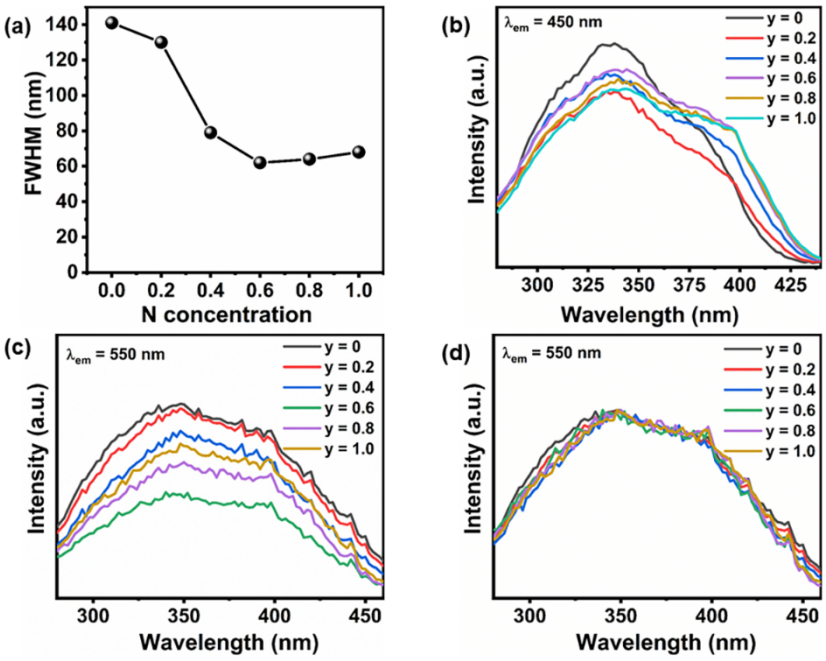

Figure S3. (a) FWHM of $BAON_y$:Eu PL spectra at the excitation wavelength of 400 nm. (b) PLE spectra of $BAON_y$:Eu at the monitoring wavelength of 450 nm. (c) PLE spectra of $BAON_y$:Eu at the monitoring wavelength of 550 nm. (d) Normalized PLE spectra of $BAON_y$:Eu at the monitoring wavelength of 550 nm.

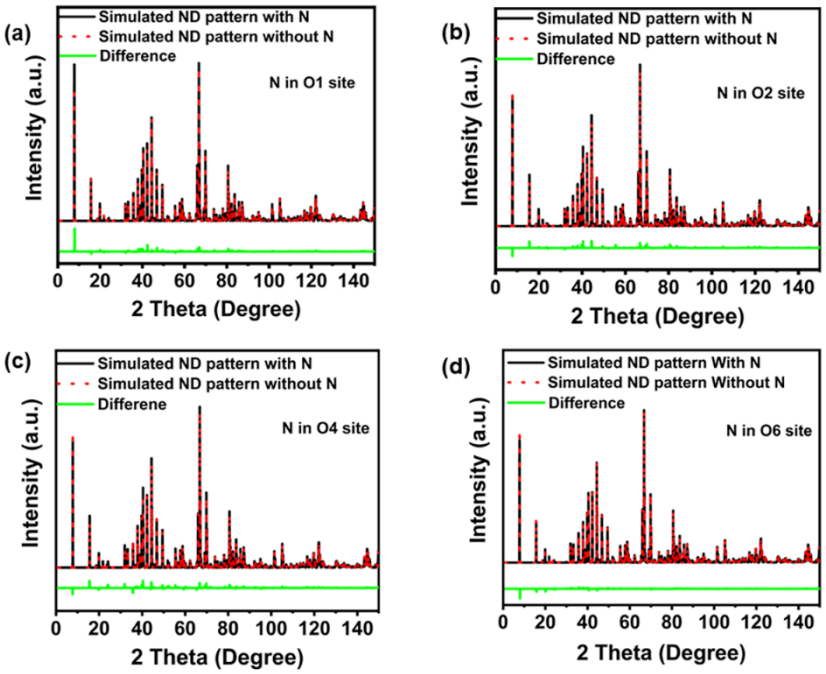

Figure S4. (a-d) Simulated ND patterns comparison between N element in different O sites. The doping ratio of N^{3-} in simulating process was based on y = 1.0.

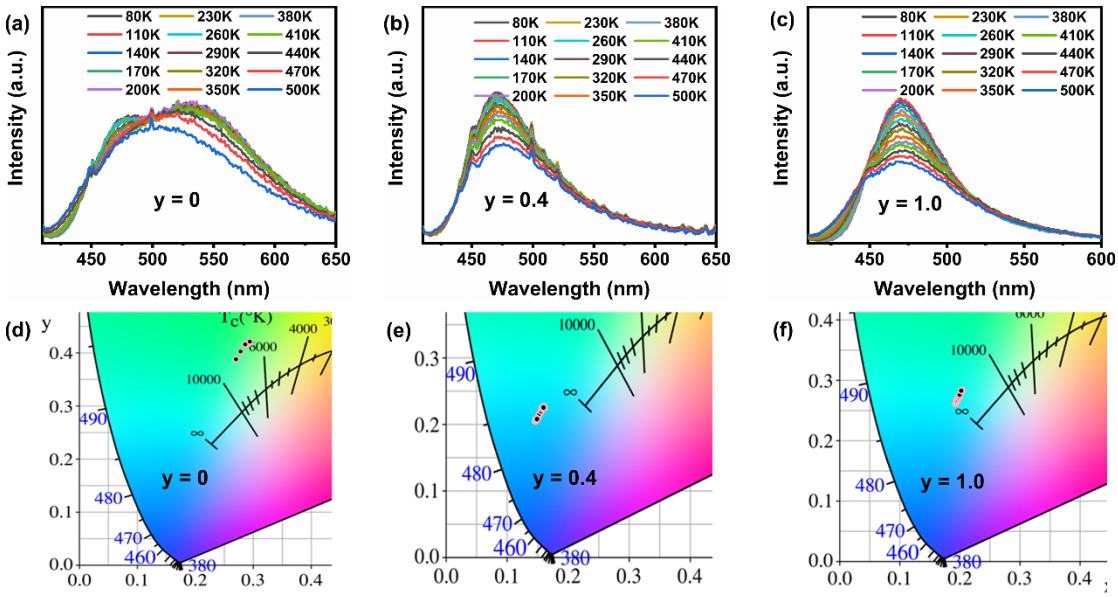

Figure S5. Temperature-dependent PL spectra of $BAON_y$:Eu phosphors at (a) y = 0, (b) 0.4 and (c) 1.0 as well as the corresponding CIE coordinates at (d) y = 0, (e) 0.4 and (f) 1.0.

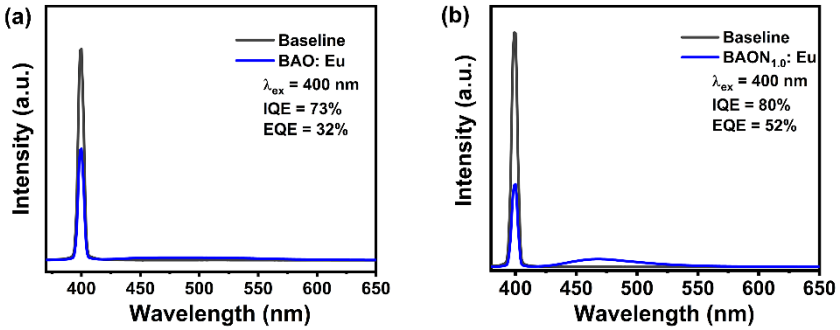

Figure S6. QE of BAO:Eu and $BAON_{1.0}$:Eu at the excitation of 400 nm light, respectively.

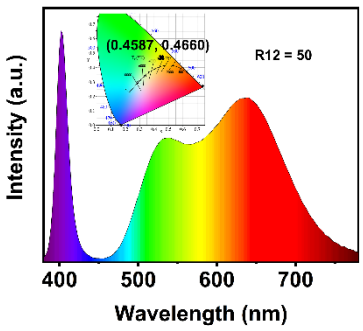

Figure S7. EL spectrum of packaged LED with violet chip and $(Sr,Ba)_2SiO_4$:Eu, Sr_3SiO_5:Eu, $CaAlSiN_3$:Eu phosphors.