

Supporting Information

**Dual-Site Occupancy Induced Broadband Cyan Emission in
 $\text{Ba}_2\text{CaB}_2\text{Si}_4\text{O}_{14}:\text{Ce}^{3+}$**

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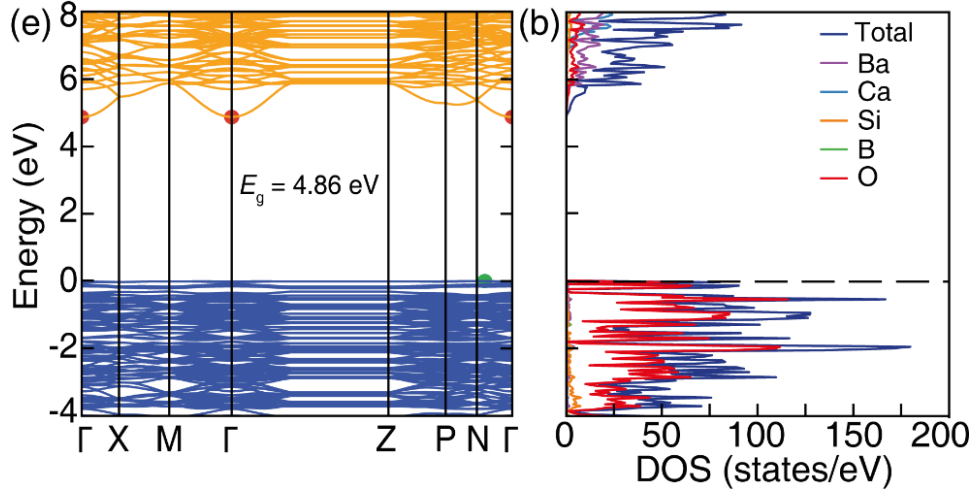


Figure S1. (a) The band structure and (b) projected total density of states (DOS) of BCBSO host calculate with the DFT-PBE method.

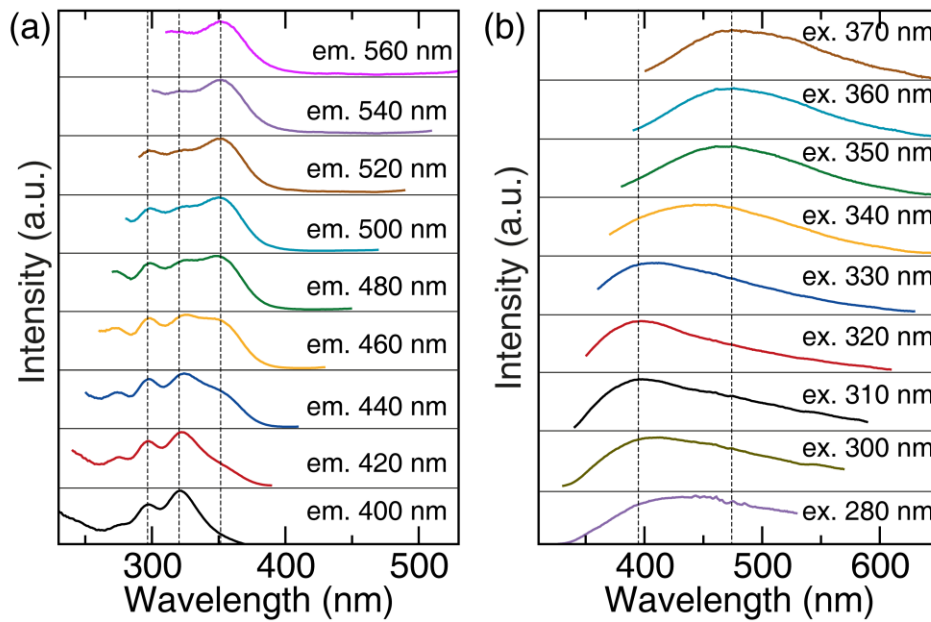


Figure S2. (a) Photoluminescence excitation spectra monitored at different emission wavelengths and (b) emission spectra recorded under different excitation wavelengths of BCBSO:0.03Ce³⁺.

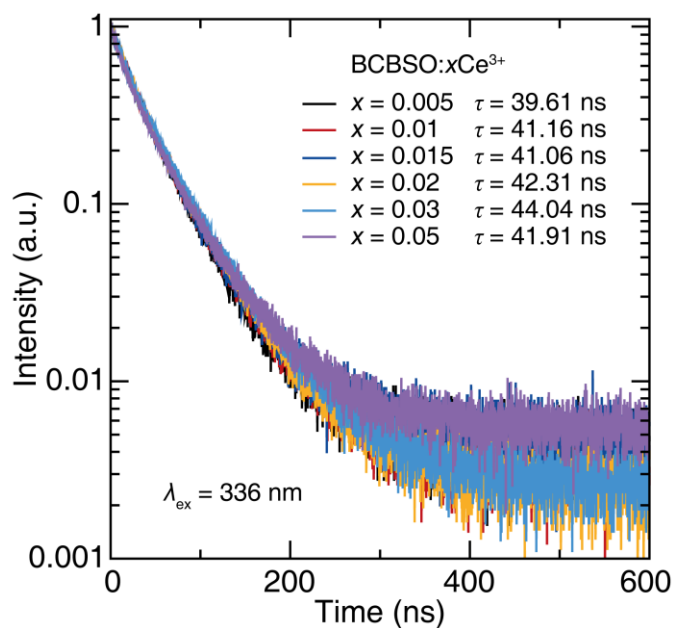


Figure S3. Decay curves of BCBSO: $x\text{Ce}^{3+}$ ($x = 0.005 - 0.05$) samples under 336 nm excitation.

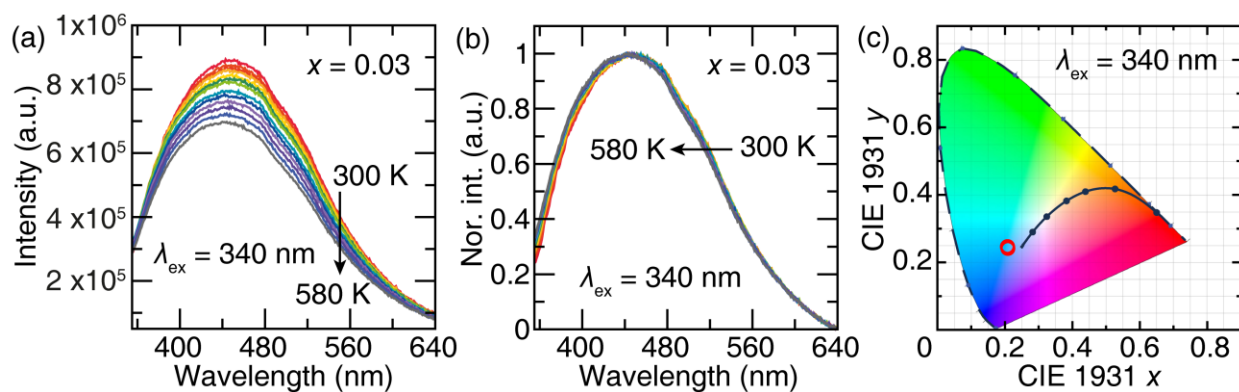


Figure S4. (a) Emission spectra, (b) normalized emission spectra, and (c) CIE 1931 chromaticity coordinates of BCBSO:0.03 Ce^{3+} versus temperature ranging from 300 to 580 K under a 340 nm light excitation.

Table S1. Refine atom positions, thermal parameters, and occupancies of Ba₂CaB₂Si₄O₁₄ from the Rietveld refinement of high-resolution synchrotron XRD data.

atom	Wyck. pos.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} (Å ²)	occ.
Ba1	8 <i>i</i>	0.20563(6)	0.20563(6)	0.99925(1)	0.00964	1
Ca1	4 <i>e</i>	0	0	0.24435(9)	0.00067	1
Si1	16 <i>j</i>	0.51415(2)	0.20096(5)	0.23648(9)	0.00403	1
B1	8 <i>g</i>	0.50000(0)	0.33241(9)	0	0.00364	1
O1	8 <i>i</i>	0.40626(5)	0.40626(5)	0.06633(2)	0.00186	1
O2	16 <i>j</i>	0.56000(4)	0.25457(8)	0.09906(3)	0.00055	1
O3	16 <i>j</i>	0.49488(4)	0.30236(9)	0.34550(9)	0.00471	1
O4	16 <i>j</i>	0.62426(1)	0.11044(8)	0.28914(5)	0.00516	1

Table S2. Emission peaks (λ_{em}) and the full width at half maximum (FWHM) of BCBSO:0.03Ce³⁺ under different excitation wavelengths (λ_{ex}).

λ_{ex} (nm)	λ_{ex} (nm)	FWHM (nm; cm ⁻¹)
310	395	146 (8053)
320	399	121 (7022)
330	410	138 (7624)
340	455	161 (8010)
350	478	142 (6053)
360	479	135 (5792)
370	480	133 (5539)

Table S3. Luminescent decay component (τ_1 , τ_2) and corresponding percentage contributions (%), and the average lifetime (τ_{av}) of BCBSO: $x\text{Ce}^{3+}$ ($x = 0.005 - 0.05$) under 336 nm excitation.

x	τ_1 (ns)	Percent. (%)	τ_2 (ns)	Percent. (%)	τ_{av} (ns)	R^2_{adj}
0.005	21.33	42	45.85	58	39.61	0.9992
0.01	20.20	41	47.39	59	41.16	0.9995
0.015	18.80	40	47.08	60	41.06	0.9992
0.02	18.51	38	47.96	62	42.31	0.9996
0.03	19.00	38	49.93	62	44.04	0.9996
0.05	15.07	39	47.37	61	41.91	0.9991

Table S4. Color rendering indexes of wLED-1 and wLED-2 using BCBSO:0.03Ce³⁺ as cyan phosphor.

Devices	R_a	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	R_9	R_{10}	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}
wLED-1	91	92	91	89	92	92	88	92	95	96	78	90	85	91	94	95
wLED-2	95	97	97	97	96	97	93	94	90	75	94	91	93	96	98	97