Broadband photoluminescence toward NIR II region and stable green ceramic pigments based on a novel $NaBaScSi_2O_7$: xCr silicate phosphor

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Table S1. A comparison of the luminescent properties of Cr^{3+}-activated broadband NIR phosphors with those of this work.

Phosphor	λ_{em}/nm	λ_{em}/nm	FWHM/nm	$I@T$/°C	Refs.
Emission wavelengths in NIR-I region (650-900 nm)					
$La_3Sc_2Ga_3O_{12}$: Cr^{3+}	480	818	145	<60%@150	[1]
$LiInP_2O_7$: Cr^{3+}	460	860	165	2.2%@100	[2]
$ScBO_3$: Cr^{3+}	450	800	120	49%@150	[3]
$BaSnSi_3O_9$: Cr^{3+}	449	806	162	38%@150	[4]
K_3GaF_6: Cr^{3+}	442	750	140	<50%@50	[5]
$Sr_8MgLa(PO_4)_7$: Cr^{3+}	490	870	140	≈15%@150	[6]
$LiScP_2O_7$: Cr^{3+}	470	880	170	20%@150	[7]
$CaSc_2O_4$: Cr^{3+}	470	819	170	≈35%@150	[8]
$CaMgGe_2O_6$: Cr^{3+}	450	845	160	≈50%@150	[9]
$Ca_3Sc_2Si_3O_{12}$: Cr^{3+}	460	770	100	50%@150	[10]
$Lu_2CaMg_2Ge_3O_{12}$: Cr^{3+}	455	795	152	67.1%@150	[11]
$Y_{0.57}La_{0.72}Sc_{2.71}(BO_3)_4$: Cr^{3+}	466	850	172	41%@100	[12]
$NaScGe_2O_6$: Cr^{3+}	490	895	162	20%@150	[13]
$SrGa_2O_4$: Cr^{3+}	420	700	170	56%@150	[14]
$LiScSi_2O_6$: Cr^{3+}	460	845	156	75%@150	[15]
$Sr_9Ga(PO_4)_7$: Cr^{3+}	485	848	150	<5%@150	[16]
$K_6Li_{0.9}Na_{0.1}CaSc_2(B_5O_{10})_3$: Cr^{3+}	465	825	167	50%@125	[17]
$GaTaO_4$: Cr^{3+}	470	825	127	74%@100	[18]
Emission wavelengths toward NIR-II region (>900 nm)					
$InTaO_4$: Cr^{3+}	510	975	196	<5%@150	[18]
$CaSc_{0.85}Al_{1.15}SiO_6$: Cr^{3+}	460	950	205	47%@100	[19]
$NaInGe_2O_6$: Cr^{3+}	460	935	170	43%@150	[20]
$LiSc_{0.5}Ga_{0.5}W_2O_8$: Cr^{3+}	524	998	200	<40%@150	[21]
$LiIn_2SbO_6$: Cr^{3+}	460	965	217	<10%@150	[22]
$Cs_2NaInCl_6$: Cr^{3+}	290	958	165	-	[23]
$ZnWO_4$: Cr^{3+}	520	987	212	-	[24]
$NaBaScSi_2O_7$: Cr^{3+}	493	974	140	51%@150	This work

Table S2. Experimental parameters of powder XRD and refined crystallographic data for $NaBaSc_{0.95}Si_2O_7$: $0.05Cr^{3+}$.

Chemical Formula	$NaBaSc_{0.95}Si_2O_7$: $0.05Cr^{3+}$
Diffractometer	Model Ultima IV
Radiation type	Cu Kα, λ = 1.54060 Å
2θ interval (°)	5.00-100.00
Step size of 2θ (°)	0.01
Space group	$P2_1/m$
a (Å)	6.84649(9)
b (Å)	5.62458(7)
c (Å)	8.81783(13)
α (°)	90
β (°)	109.2808(11)
γ (°)	90
V (Å^3)	320.5171(79)
$^b R_p$ (%)	8.73
$^c R_{wp}$ (%)	5.76
R_{exp} (%)	3.11
^{d} S	2.80

$$^bR_P = \sum\left|y_i - y_{C,i}\right| / \sum y_i \; ; \; ^cR_{wp} = \left[\sum w_i\left|y_i - Y_{C,i}\right|^2 / \sum w_i y_i^2\right]^{\frac{1}{2}} ; \; ^dS = R_{wp} / R_{exp}$$

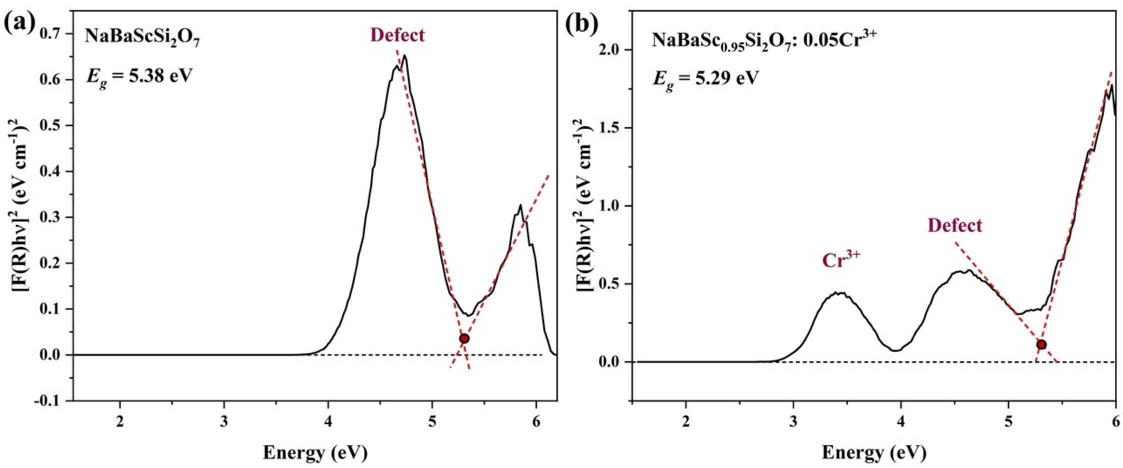

Fig. S1 The band gap determination of (a)$NaBaScSi_2O_7$ and (b) $NaBaSc_{0.95}Si_2O_7$: $0.05Cr^{3+}$.

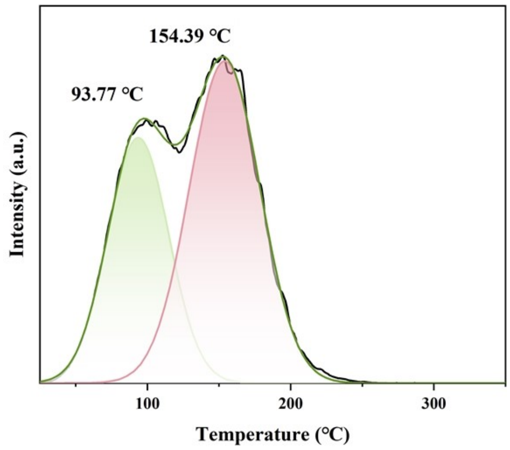

Fig. S2 Thermoluminescence analysis of the $NaBaScSi_2O_7$.

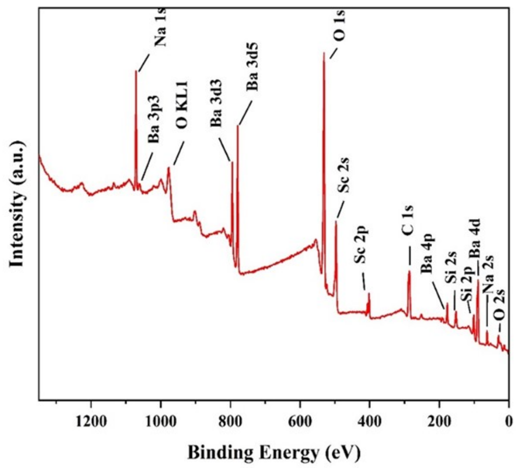

Fig. S3 The XPS spectrum of $NaBaSc_{0.95}Si_2O_7$: $0.05Cr^{3+}$.

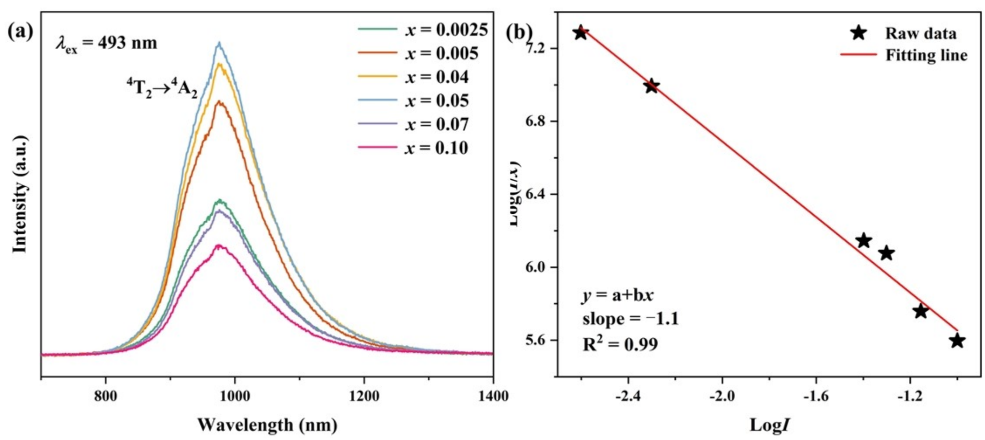

Fig. S4 (a) The PL spectra of $NaBaSc_{1-x}Si_2O_7$: xCr^{3+}, (b) linear fit of the relationship between log(I/x) and log$x$.

The critical energy transfer distance R_c between activators is calculated using Blasse's equation: [25]

$$R_c \approx 2\left(\frac{3V}{4\pi X_c N}\right)^{1/3} \quad (1)$$

where V is the volume of the crystallographic unit cell, X_c is the critical concentration, and N is the number of cationic sites per unit cell replaced by activators. The volume V, the number of cations per unit cell N, and the critical concentration X_c are 320.5171 Å^3, 2, and 0.05, respectively. The type of the electric multipole interactions can be determined using the following formula: [26]

$$\frac{I}{x} = \frac{k}{1 + \beta(x)^{\theta/3}} \quad (2)$$

where I is the emission intensity, x is the content of Cr^{3+}, k and β are constants, and θ is determined by the mode of the multipole-multipole interaction, namely, non-radiative energy transfer between neighboring activator ions (θ = 3), dipole-dipole (θ = 6), dipole-quadrupole (θ = 8), or quadrupole-quadrupole (θ = 10).

Table S3. The results of fluorescence decay fitting for the 974 nm emission of the $NaBaSc_{1-x}Si_2O_7$: xCr^{3+} phosphor.

x	λ_{em} (nm)	A_1	A_2	τ_1	τ_2	χ^2	Lifetime (μs)
0.0025	974	173301.75	-168787.59	97.40	97.43	1.011	96.26
0.005	974	4699.73	66.21	89.43	239.43	1.178	94.88
0.04	974	2954.21	1925.70	55.04	95.85	1.025	76.74
0.05	974	2854.76	2070.81	52.17	93.77	1.063	75.71
0.07	974	2324.43	2173.69	42.63	86.97	1.013	71.72
0.10	974	2231.09	2350.65	47.68	89.86	0.942	75.73

Table S4. The results of fluorescence decay fitting for the 974 nm emission of the $NaBaSc_{0.95}Si_2O_7$: $0.05Cr^{3+}$ phosphor at different temperature.

Temperature	λ_{em} (nm)	A_1	A_2	τ_1	τ_2	χ^2	Lifetime (μs)
RT	974	2854.76	2070.81	52.17	93.77	1.063	75.71
323 K	974	3770.58	1183.66	57.15	102.96	0.995	73.70
348 K	974	3522.25	1368.54	53.79	93.28	0.981	69.69
373 K	974	4215.74	685.7	53.32	102.7	0.995	65.10
398 K	974	4187.34	573.76	49.55	93.6	1.027	58.61
423 K	974	4262.29	454.56	43.74	81.71	1.033	50.05
448 K	974	5027.28	14.05	38.91	190.78	1.075	40.96
473 K	974	5062.61	1.23	30.29	500	1.049	32.17
498 K	974	-606.18	5585.33	10.02	22.09	1.068	22.71
523 K	974	-404.01	5249.23	1.33	16.54	0.970	16.63

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