Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The Photoluminescence, Thermal Properties and Tunable Color of $Na_{1-x}Al_{1+2x}Si_{1-2x}O_4:xCe^{3+}/Tb^{3+}/Dy^{3+}$ via Energy Transfer: A Single-Component Multicolor-Emitting Phosphor

Chengyi Xu,[a] Yanhua Song,[a] Hongxia Guan,[a] Ye Sheng,[a] Pingchuan Ma,[a] Xiuqing Zhou,[a] Zhan Shi[b] and Haifeng Zou*[a]

[a] College of chemistry, Jilin University, Changchun 130012, PR China.

[b] State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, PR China

Telephone: +86-0431-85155275; Fax: +86-0431-85155275; E-mail: zouhf@jlu.edu.cn

Table S1 Crystal structural data and lattice parameters of NAS:Ce^{3+}/Tb^{3+}/Dy^{3+}

Formula	Crystal system	Space group	Lattice parameters				Reliability factors		
			a=b/Å	c/Å	α=β/°	γ/°	R_p/%	R_{wp}/%	χ^2
$Na_{0.99}Al_{1.02}Si_{0.98}O_4$:0.01$Dy^{3+}$	Hexagonal	P63(173)	9.98	8.35	90	120	5.99	7.95	1.83
$Na_{0.98}Al_{1.04}Si_{0.96}O_4$:0.02$Tb^{3+}$	Hexagonal	P63(173)	9.98	8.35	90	120	5.65	7.37	1.67
$Na_{0.97}Al_{1.06}Si_{0.94}O_4$:0.02$Ce^{3+}$,0.01$Dy^{3+}$	Hexagonal	P63(173)	9.98	8.35	90	120	6.66	8.66	2.07
$Na_{0.97}Al_{1.06}Si_{0.94}O_4$:0.02$Ce^{3+}$,0.01$Tb^{3+}$	Hexagonal	P63(173)	9.98	8.35	90	120	6.67	8.66	1.91

Table S2 Atomic coordinates and site occupancy fraction (SOF) for $Na_{0.98}Al_{1.04}Si_{0.96}O_4$:2%$Tb^{3+}$.

Atom	x	y	z	SOF
Na1	-0.000934	0.452933	-0.000061	0.9812
Tb1	-0.000934	0.452933	-0.000061	0.0188
Na2	0	0	0.052904	1
Al1	1/3	2/3	0.178312	1
Al2	0.095145	0.329542	0.690720	1
Si1	1/3	2/3	0.812628	0.9699
Al3	1/3	2/3	0.812628	0.0301
Si2	0.098304	0.340726	0.312907	0.9628
Al4	0.098304	0.340726	0.312907	0.0372
O1	1/3	2/3	-0.012604	1
O2	0.024393	0.309930	0.490421	1
O3	0.163312	0.475699	0.719878	1
O4	0.185133	0.533738	0.263456	1
O5	0.253060	0.250932	0.311403	1
O6	0.221038	0.280080	0.697272	1

Table S3 Atomic coordinates and site occupancy fraction (SOF) for $Na_{0.99}Al_{1.02}Si_{0.98}O_4$:1%$Dy^{3+}$.

Atom	x	y	z	SOF
Na1	-0.010411	0.444126	-0.010470	0.9903
Dy1	-0.010411	0.444126	-0.010470	0.0097
Na2	0	0	0.060912	1
Al1	1/3	2/3	0.205199	1
Al2	0.096945	0.338543	0.689343	1
Si1	1/3	2/3	0.834405	0.9822
Al3	1/3	2/3	0.834405	0.0178
Si2	0.098876	0.332811	0.315023	0.9815
Al4	0.098876	0.332811	0.315023	0.0185
O1	1/3	2/3	0.028817	1
O2	0.026739	0.316361	0.496476	1
O3	0.185399	0.528434	0.744194	1
O4	0.159979	0.476619	0.277919	1
O5	0.219622	0.276217	0.315951	1
O6	0.254801	0.250810	0.703103	1

Table S4 Atomic coordinates and site occupancy fraction (SOF) for $Na_{0.97}Al_{1.06}Si_{0.94}O_4$:2%Ce, 1%$Tb^{3+}$.				
Atom	**x**	**y**	**z**	**SOF**
Na1	-0.005610	0.446649	-0.008492	0.9717
Ce1	-0.005610	0.446649	-0.008492	0.0193
Tb1	-0.005610	0.446649	-0.008492	0.0090
Na2	0	0	0.013796	1
Al1	1/3	2/3	0.165922	1
Al2	0.098488	0.329801	0.696300	1
Si1	1/3	2/3	0.805461	0.9432
Al3	1/3	2/3	0.805461	0.0568
Si2	0.105768	0.349816	0.323283	0.9435
Al4	0.105768	0.349816	0.323283	0.0565
O1	1/3	2/3	-0.018987	1
O2	0.025102	0.307870	0.514969	1
O3	0.169463	0.474378	0.702711	1
O4	0.187080	0.541881	0.245516	1
O5	0.250815	0.253792	0.307650	1
O6	0.247052	0.272761	0.692423	1

Table S5 Atomic coordinates and site occupancy fraction (SOF) for $Na_{0.97}Al_{1.06}Si_{0.94}O_4$:2%$Ce^{3+}$, 1%$Dy^{3+}$.				
Atom	**x**	**y**	**z**	**SOF**
Na1	-0.005223	0.443249	-0.004544	0.9709
Ce1	-0.005223	0.443249	-0.004544	0.0197
Dy1	-0.005223	0.443249	-0.004544	0.0094
Na2	0	0	0.040925	1
Al1	1/3	2/3	0.173669	1
Al2	0.094235	0.327197	0.693777	1
Si1	1/3	2/3	0.799515	0.9469
Al3	1/3	2/3	0.799515	0.0531
Si2	0.119349	0.353784	0.323142	0.9450
Al4	0.119349	0.353784	0.323142	0.0550
O1	1/3	2/3	-0.025404	1
O2	0.021666	0.310215	0.496739	1
O3	0.166577	0.478467	0.708668	1
O4	0.175916	0.540717	0.251409	1
O5	0.250217	0.252528	0.314270	1
O6	0.243337	0.268654	0.699856	1

Table S6 The mass ratio of each element for different concentrations of Ce^{3+}, Tb^{3+} and Dy^{3+} ion activated NAS samples

Elements	Line	Wt%					
		NAS	NAS:2% Ce^{3+}	NAS:2% Tb^{3+}	NAS:2% Dy^{3+}	NAS:2%Ce^{3+},2% Tb^{3+}	NAS:2%Ce^{3+},2% Dy^{3+}
O	Kα	44.57	43.55	43.11	41.09	44.29	42.29
Na	Kα	16.50	15.63	15.66	15.54	15.20	15.77
Al	Kα	18.92	19.05	50.76	20.58	18.02	19.94
Si	Kα	20.01	18.04	18.50	19.43	17.52	17.18
Ce	Lα	-	3.73	-	-	2.80	3.08
Tb	Lα	-	-	1.97	-	2.17	-
Dy	Lα	-	-	-	3.36	-	1.74

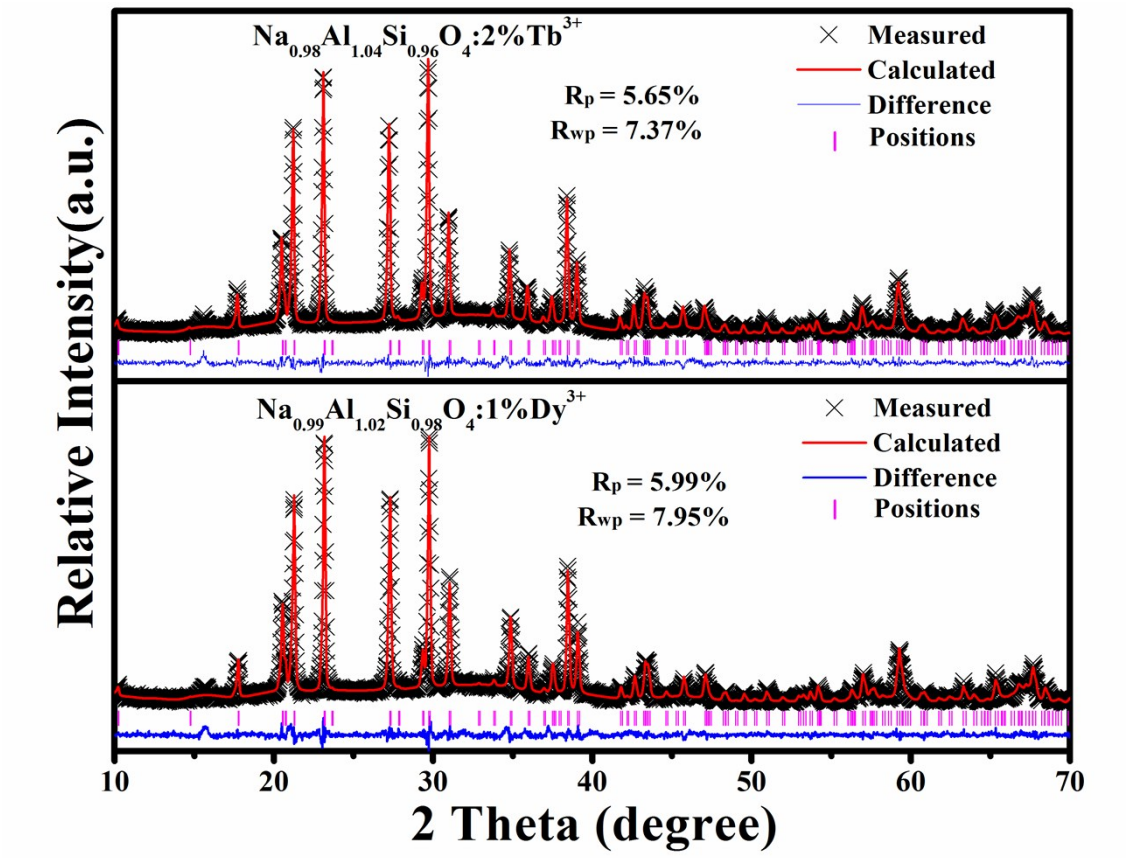

Fig.S1 Rietveld refinement of the powder XRD pattern of NAS:2%Tb^{3+} and NAS:1%Dy^{3+}.

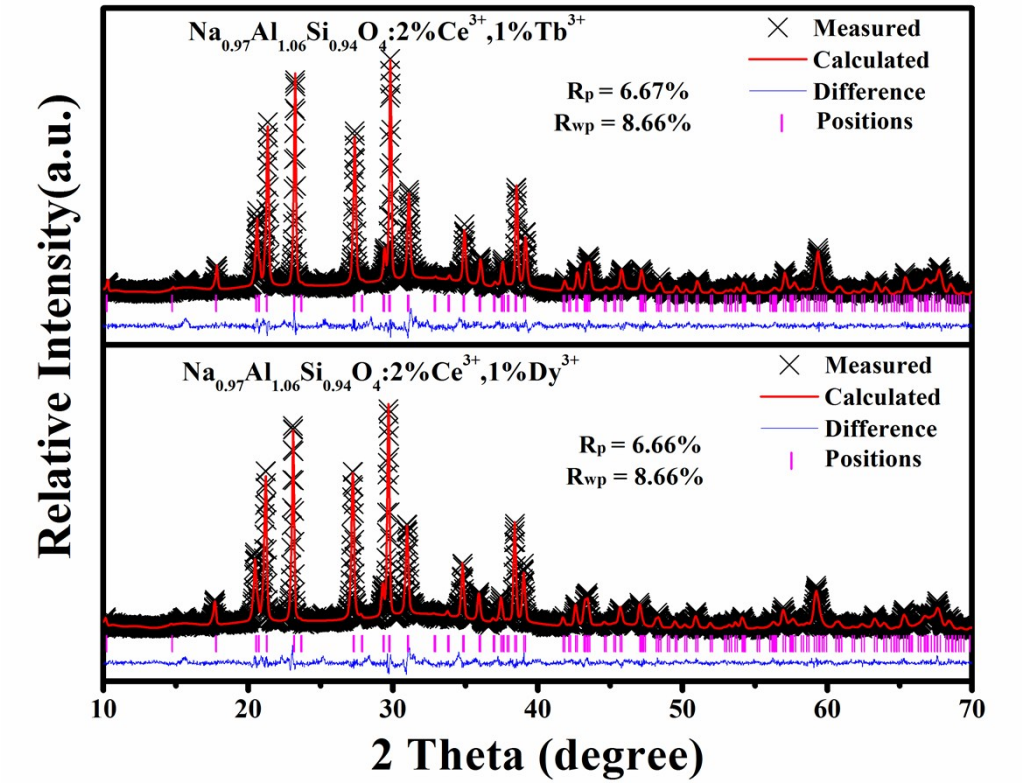

Fig.S2 Rietveld refinement of the powder XRD pattern of NAS:2%Ce^{3+},1%Tb^{3+} and NAS:2%Ce^{3+},1%Dy^{3+}.

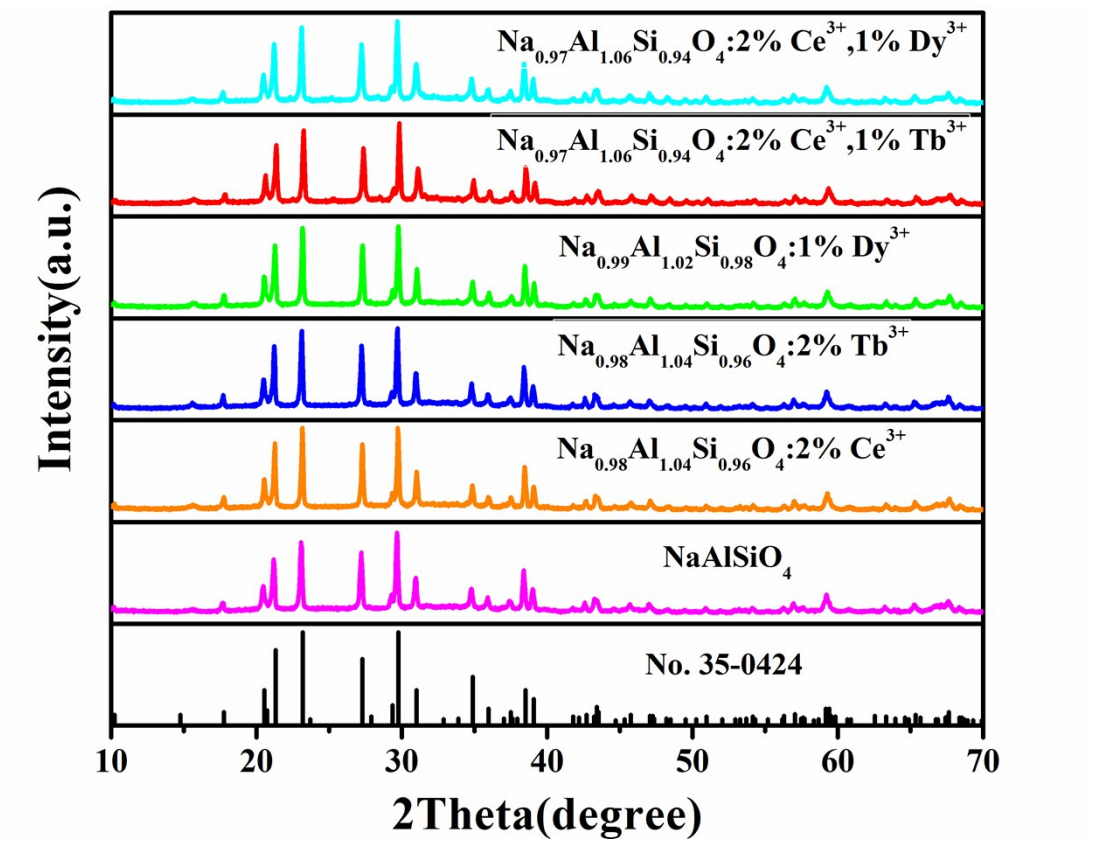

Fig.S3 The representative XRD patterns for Ce^{3+}/Tb^{3+}/Dy^{3+} doped NAS samples.

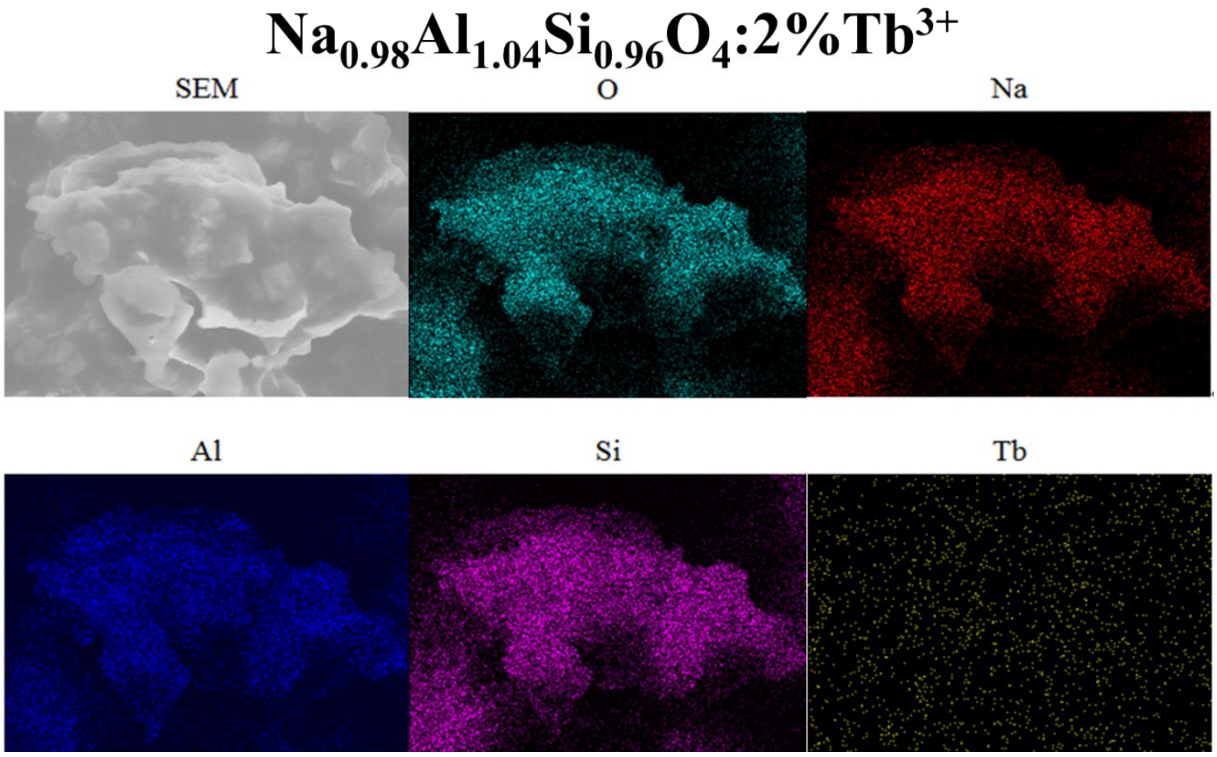

Fig.S4 The analysis of SEM and mapping for each element in NAS:2%Tb^{3+}.

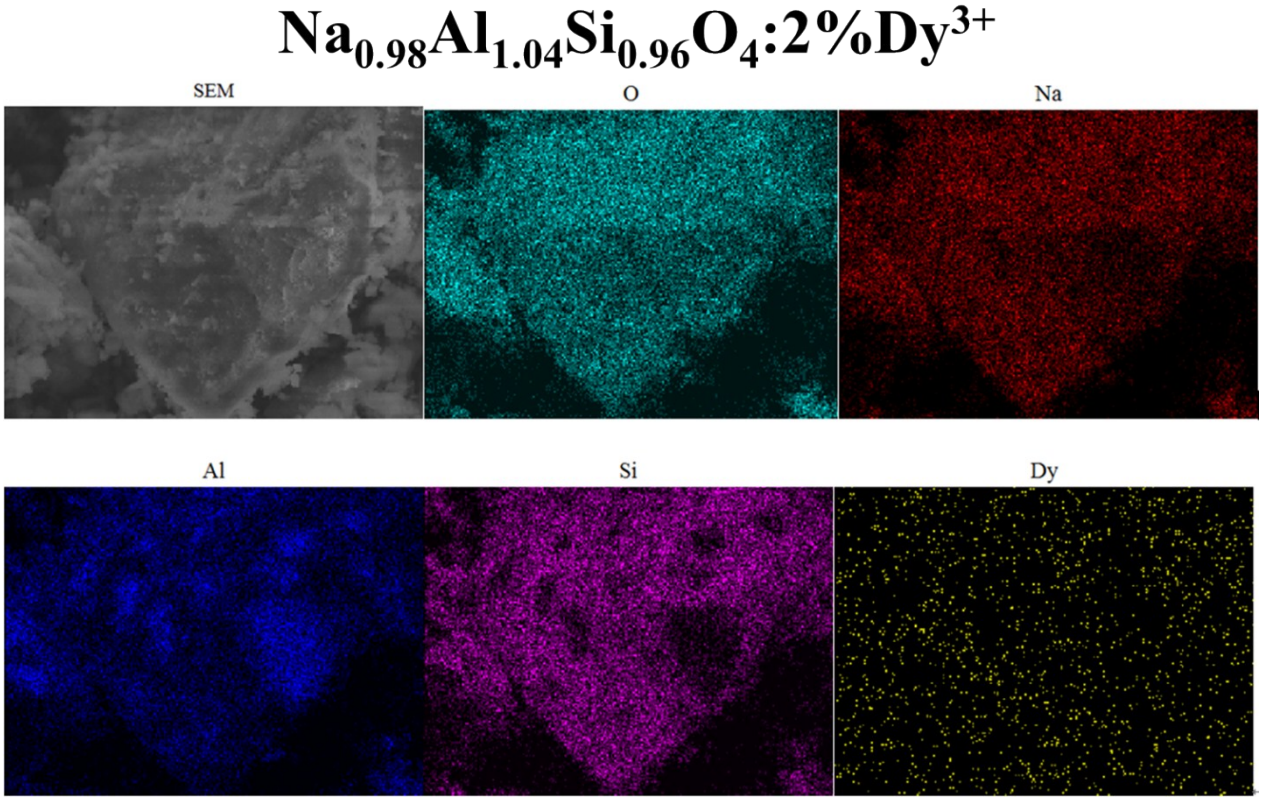

Fig.S5 The analysis of SEM and mapping for each element in NAS:2%Dy^{3+}.

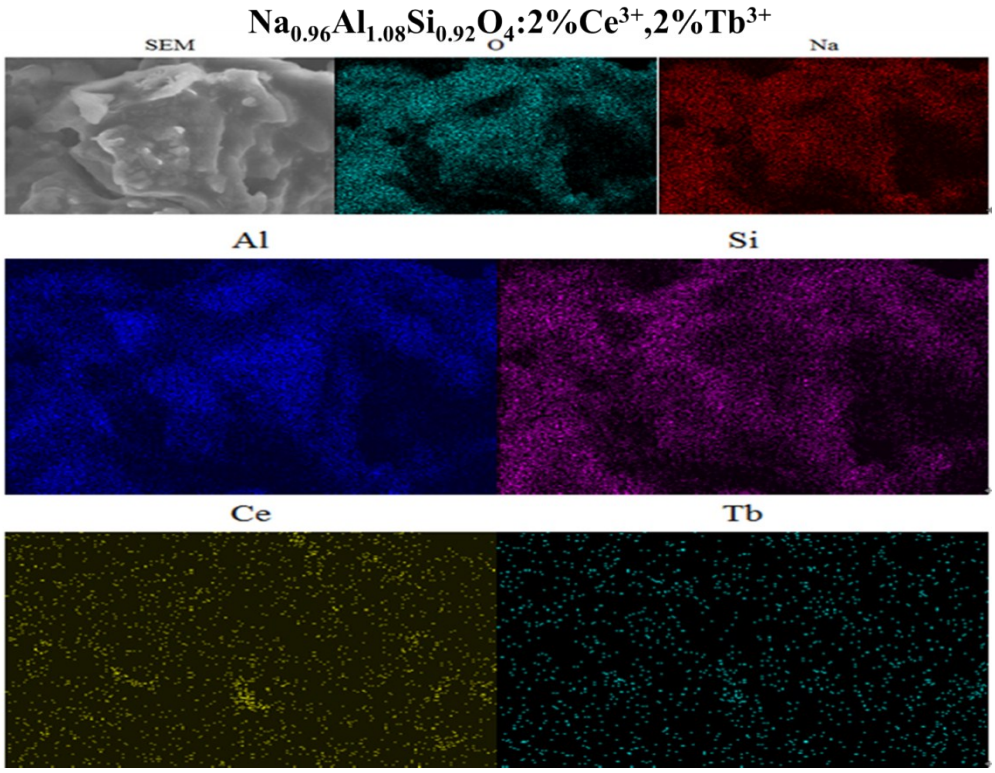

Fig.S6 The analysis of SEM and mapping for each element in NAS:2%Ce^{3+},2%Tb^{3+}.

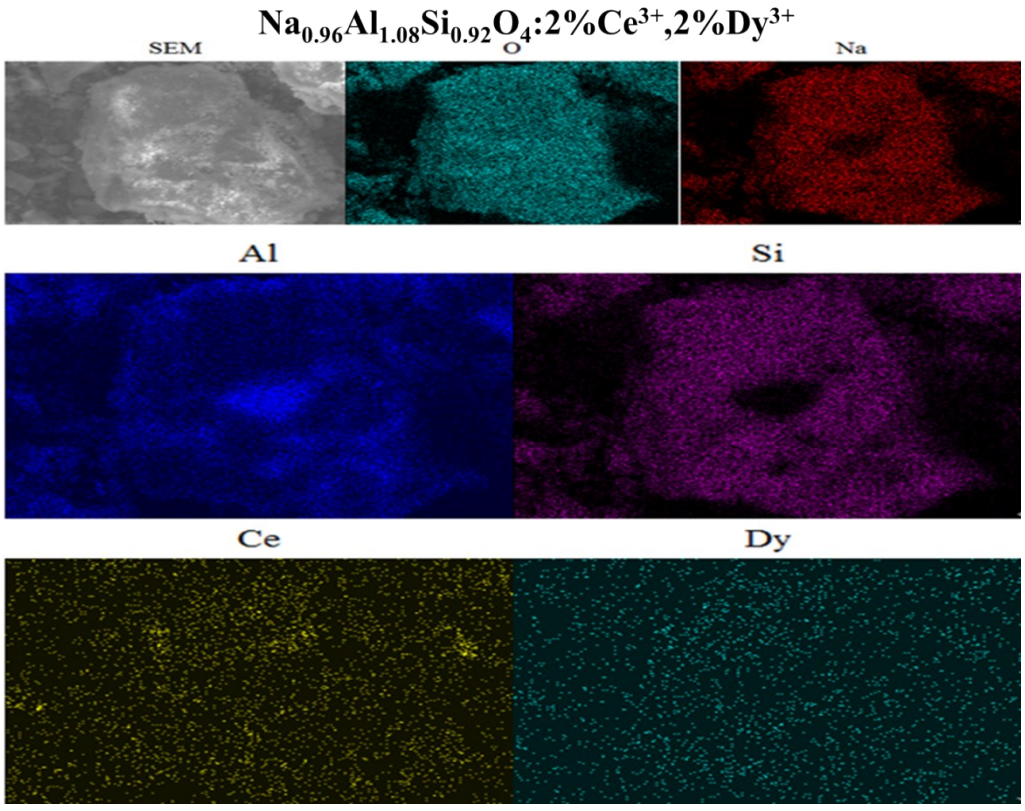

Fig.S7 The analysis of SEM and mapping for each element in NAS:2%Ce^{3+},2%Dy^{3+}.

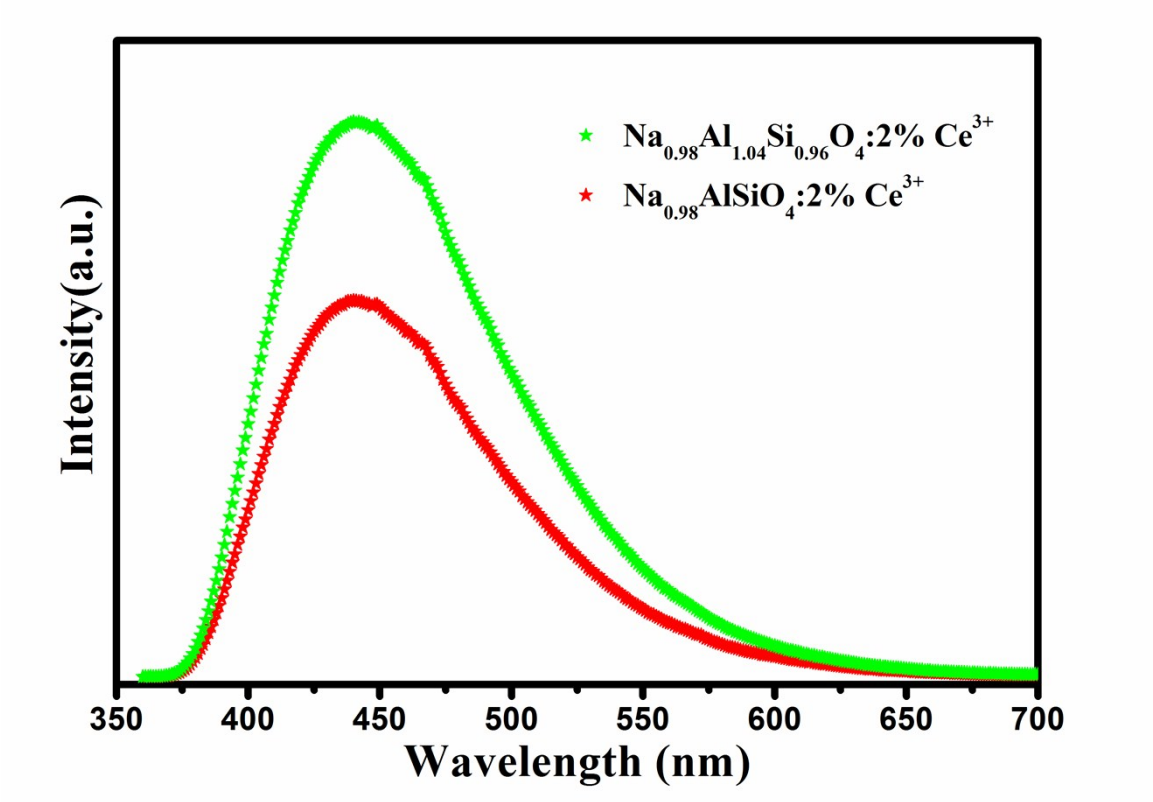

Fig. S8 The comparison of luminous intensity of NAS:2%Ce^{3+} before and after the charge compensation.

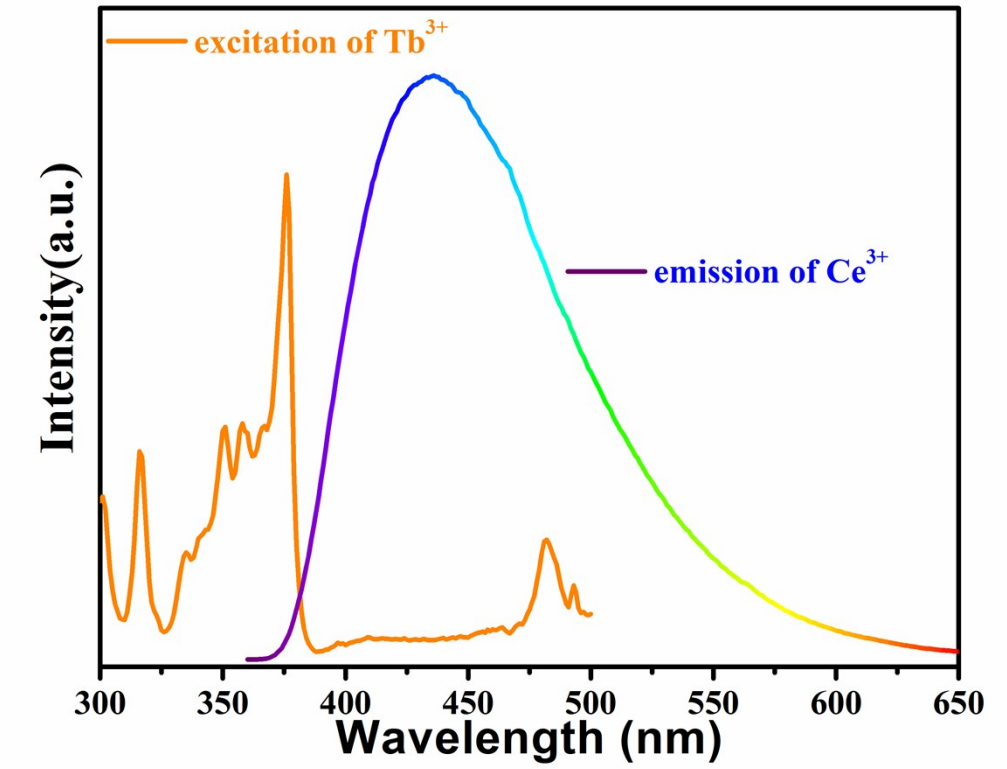

Fig.S9 Spectral overlap between the photoluminescence excitation spectrum of NAS:Tb^{3+} (orange line) and the photoluminescence spectrum of NAS:Ce^{3+} (colorized line).

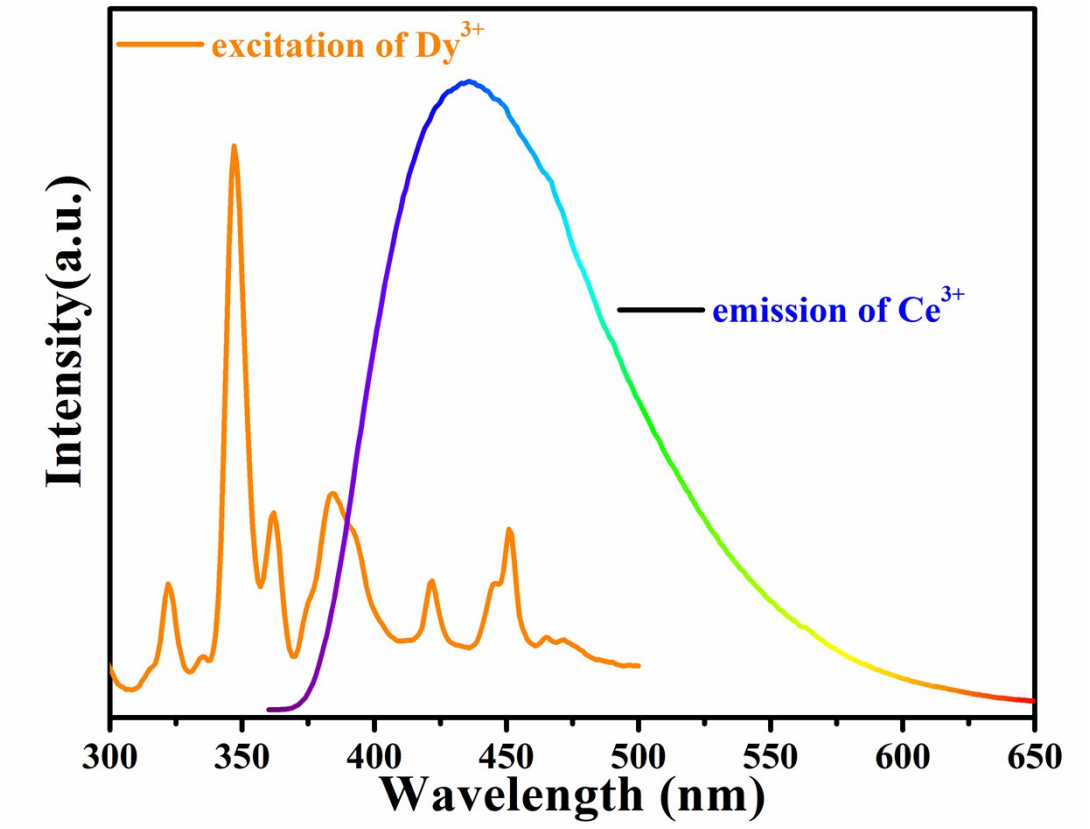

Fig.S10 Spectral overlap between the photoluminescence excitation spectrum of NAS:Dy^{3+} (orange line) and the photoluminescence spectrum of NAS:Ce^{3+} (colorized line).

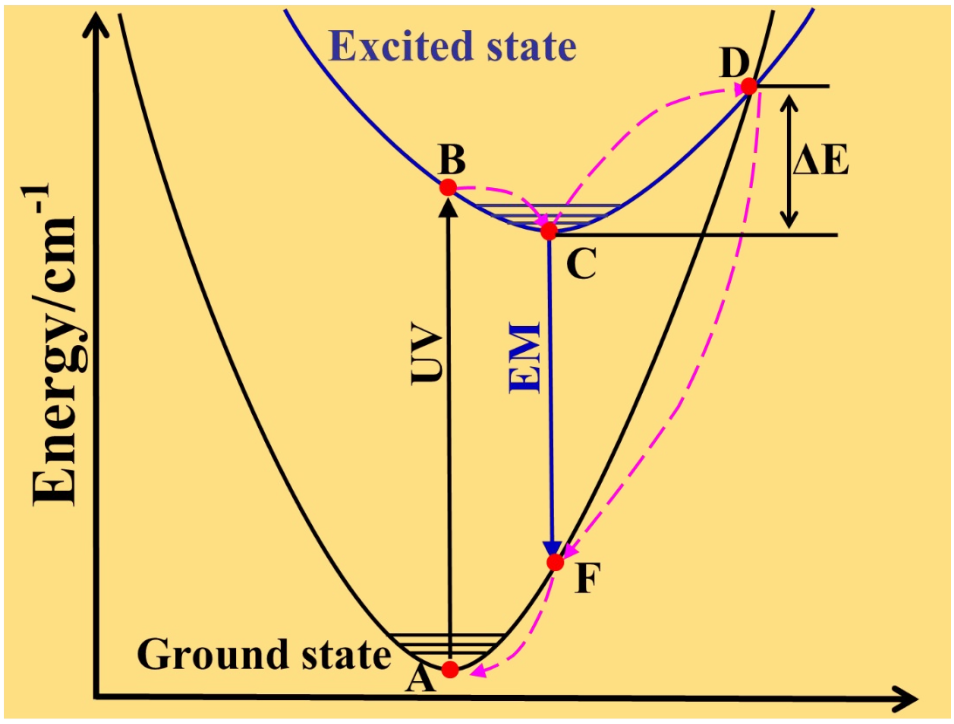

Fig.S11 The schematic of configurational coordinate diagram for general mechanism of temperature-dependent emission of phosphor.

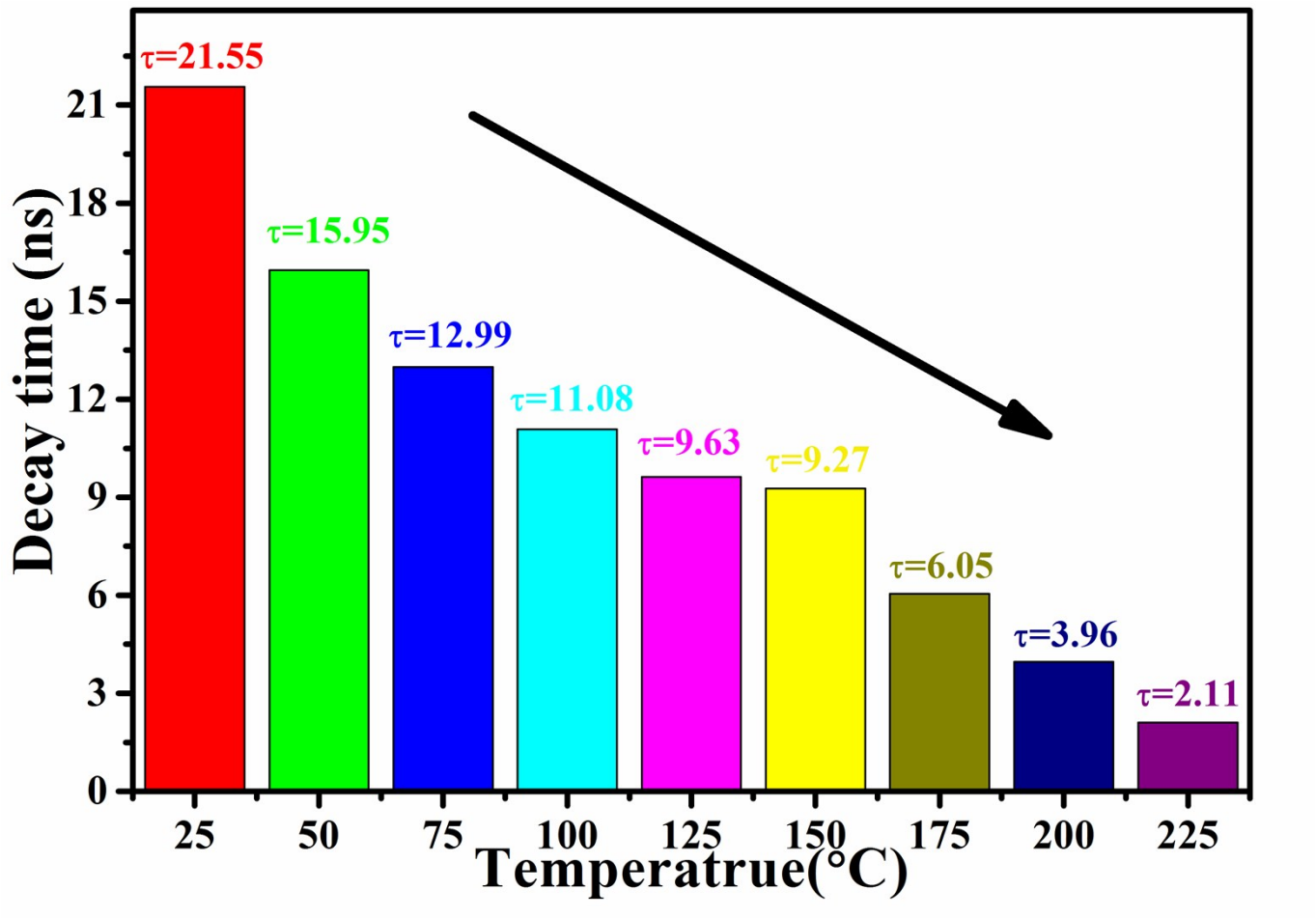

Fig.S12 The dependence of the average lifetimes (τ) on temperature for NAS:2%Ce^{3+}.