

Supporting Information

Title: Structure and photoluminescence properties of novel $\text{Ca}_2\text{NaSiO}_4\text{F}:\text{Re}$ (Re = $\text{Eu}^{2+}, \text{Ce}^{3+}, \text{Tb}^{3+}$) phosphor with energy transfer for white emitting LEDs

Author(s): Mengmeng Jiao^{a,b}, Yongchao Jia^{a,b}, Wei Lü^a, Wenzhen Lv^{a,b}, Qi Zhao^{a,b}, Baiqi Shao^{a,b}, and Hongpeng You^{a,*}

^a State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.

^b University of the Chinese Academy of Sciences, Beijing 100049, P. R. China.

*Corresponding author: E-mail: hpyou@ciac.ac.cn (H.Y.)

TableS1. Final refined structure parameters of CNSOF:0.02Eu²⁺ derived from the

Rietveld refinement of X-ray diffraction data

Atom	Wyckof f position	x	Y	z	Frac	Uiso
Ca1	8d	0.75757(3)	0.50267(3)	-0.33062(6)	0.5643	0.02445
Na1	8d	0.75757(3)	0.50267(3)	-0.33062(6)	0.4300	0.02500
Ca2	4c	0.73369(4)	0.75000(0)	-0.08830(6)	0.7722	0.01213
Na2	4c	0.73369(4)	0.75000(0)	-0.08830(6)	0.2200	0.17453
Si1	4c	0.19324(1)	0.75000(0)	0.08104(4)	1.00	0.01177
O1	8d	0.30719(4)	0.93677(2)	0.14923(1)	1.00	0.02317
O2	4c	0.30810(3)	0.75000(0)	-0.04239(7)	1.00	0.00714
O3	4c	-0.09561(5)	0.75000(0)	0.07988(0)	1.00	0.04476
F1	4c	-0.00374(6)	0.75000(0)	-0.23728(1)	1.00	0.03211
Eu1	8d	0.75757(3)	0.50267(3)	-0.33062(6)	0.0057	0.02500
Eu2	4c	0.73369(4)	0.75000(0)	-0.08830(6)	0.0078	0.02500
Cell parameters: $a = 5.3387$, $b = 7.1253$ Å, $c = 12.4407$ Å,						
$V = 473.242$ Å ³ ; $Z = 4$;						
space group: $Pnma$ (62);						
Reliability factors: $\chi^2 = 3.849$, $R_{wp} = 7.06\%$, $R_p = 5.15\%$						

TableS2. Final refined structure parameters of CNSOF:0.03Ce³⁺ derived from the

Rietveld refinement of X-ray diffraction data

Atom	Wyckof f position	x	Y	z	Frac	Uiso
Ca1	8d	0.75829(8)	0.50339(8)	-0.32990(2)	0.56145	0.01620
Na1	8d	0.75829(8)	0.50339(8)	-0.32990(2)	0.4300	0.02500
Ca2	4c	0.73431(3)	0.75000(0)	-0.08768(7)	0.7683	0.024500
Na2	4c	0.73431(3)	0.75000(0)	-0.08768(7)	0.2200	0.02500
Si1	4c	0.19561(3)	0.75000(0)	0.08294(8)	1.00	0.00374
O1	8d	0.29863(3)	0.93805(2)	0.14791(9)	1.00	0.01074
O2	4c	0.30664(3)	0.75000(0)	-0.04235(1)	1.00	0.00850
O3	4c	-0.09667(2)	0.75000(0)	0.07877(2)	1.00	0.02214
F1	4c	0.00706(8)	0.75000(0)	-0.23898(0)	1.00	0.04212
Ce1	8d	0.75829(8)	0.50339(8)	-0.32990(2)	0.00855	0.02500
Ce2	4c	0.73431(3)	0.75000(0)	-0.08768(7)	0.0117	0.02500

Cell parameters: $a = 5.3371$, $b = 7.1273$ Å, $c = 12.4374$ Å,
 $V = 473.101$ Å³; $Z = 4$;
space group: $Pnma$ (62);
Reliability factors: $\chi^2 = 3.274$, $R_{wp} = 6.57\%$, $R_p = 4.90\%$

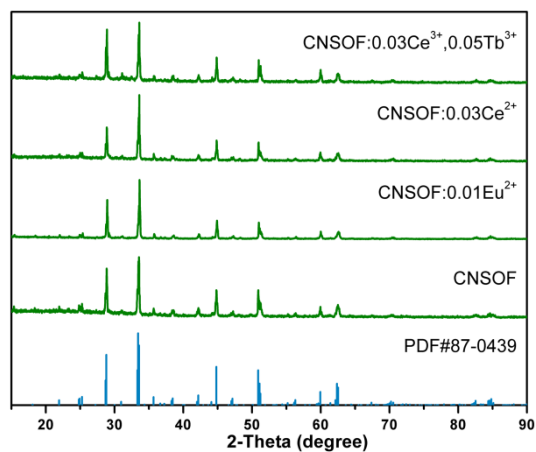


Figure S1. XRD patterns of typical prepared samples together with the standard data for reference.

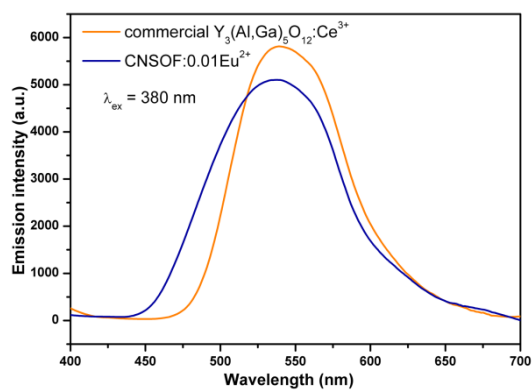


Figure S2. Emission spectra of CNSOF:0.01Eu²⁺ and $Y_3(Al,Ga)_5O_{12}:Ce^{3+}$ phosphors under same condition.

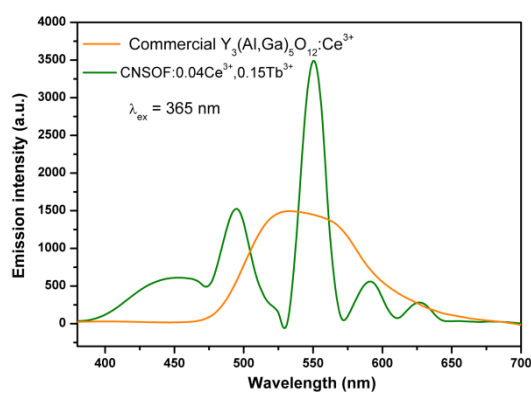


Figure S3 Emission spectra of CNSOF:0.04Ce³⁺,0.15Tb³⁺ and Y₃(Al,Ga)₅O₁₂:Ce³⁺ phosphors under same condition.

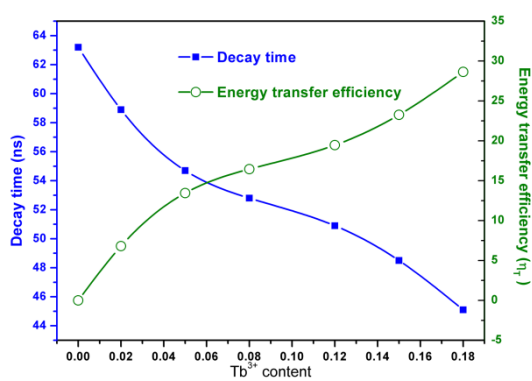


Figure S4. Decay time and energy transfer efficiency for CNSOF:0.03Ce³⁺,zTb³⁺ phosphors with different Tb³⁺ content.