Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Multiple Anti-counterfeiting Guarantees from Simple $CaTiO_3:Pr^{3+}$, Er^{3+} Particles– Multicolor Luminescence and a Multistate Luminescence Mode

Zhenbin Wang[1], Pengxiang Pei[1], Dongjie Bai[1], Shanshan Zhao[1], Xinyu Ma[1], Weisheng Liu*[1]

1, Key Laboratory of Nonferrous Metal Chemistry and Resources Utilization of Gansu Province and State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, 730000, China

Corresponding author: liuws@lzu.edu.cn

Tel.: +86 / (0) 931-8915151

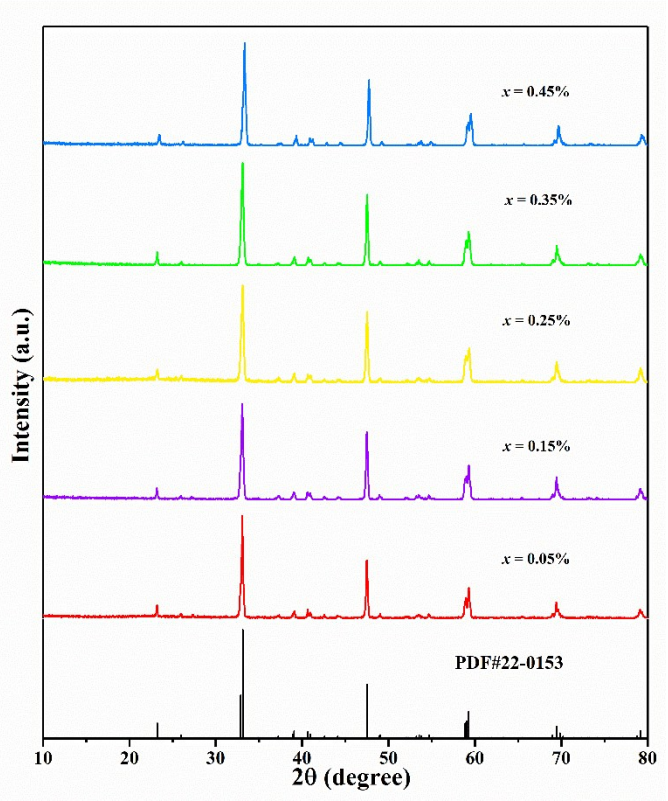

Fig. S1. XRD patterns of synthesized $CaTiO_3:xPr^{3+}$ ($0.0005 \leqslant x \leqslant 0.0045$) samples.

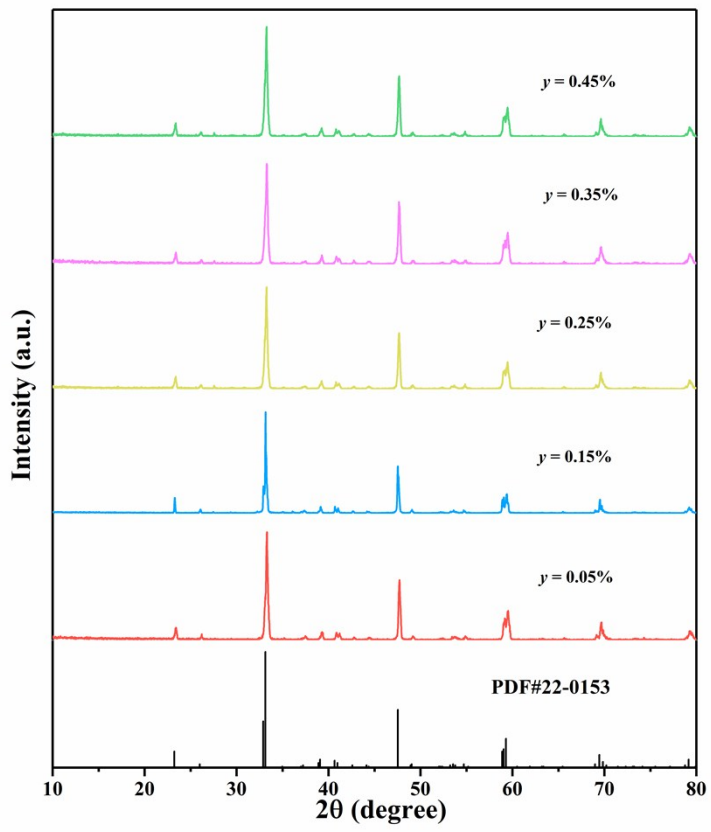

Fig. S2. XRD patterns of synthesized $CaTiO_3$:0.0025Pr^{3+}, $y$$Er^{3+}$ (0.0005$\leqslant$ y $\leqslant$0.0045) samples.

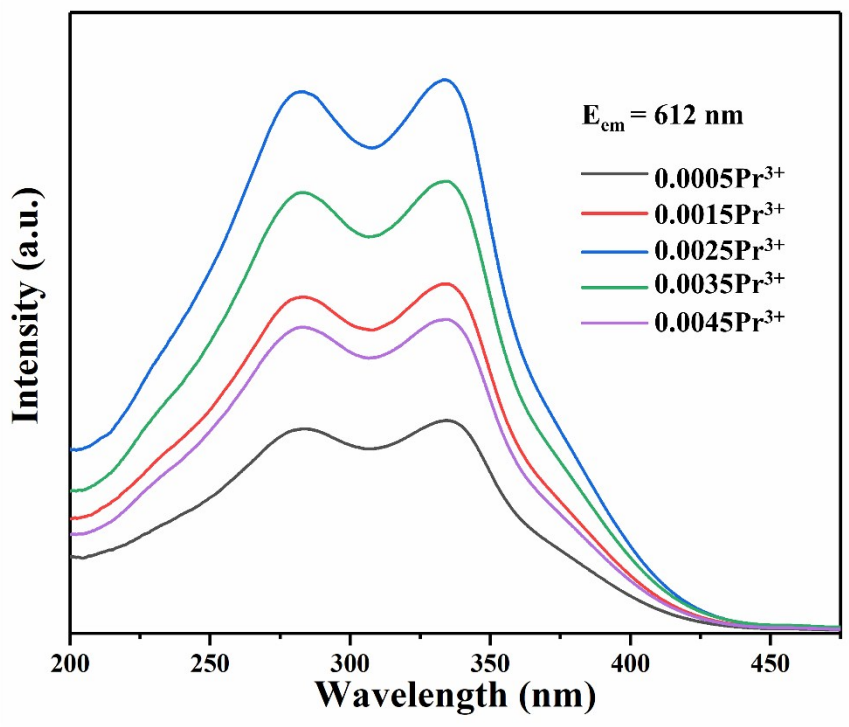

Fig. S3. Excitation spectra of $Ca_{1-x}TiO_3$:xPr^{3+}(0.0005≤x≤0.0045).

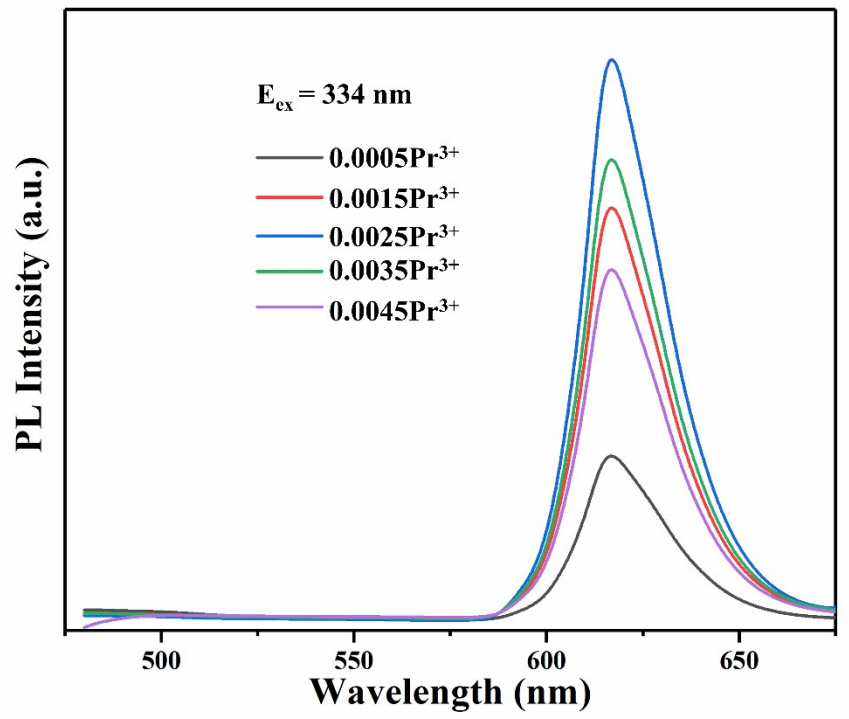

Fig. S4. Emission spectra of $Ca_{1-x}TiO_3$:xPr^{3+}(0.0005≤x≤0.0045) showing variation of

emission intensity as a function of Pr^{3+} concentrations, λ_{ex}=334nm. The optimal dopant concentration is found to be 0.25mol%, beyond which concentration quenching occurs and the emission intensity decreases dramatically[2].

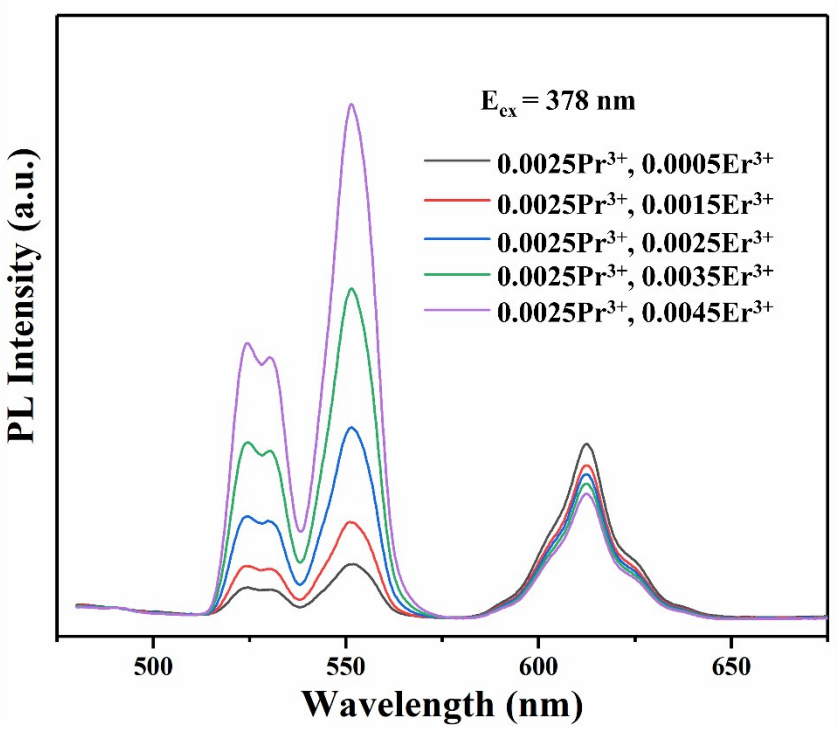

Fig. S5. Emission spectra of Pr^{3+} and Er^{3+} (λ_{ex} = 378 nm), showing an improved emission of Er^{3+} as increasing Er^{3+} concentration. Thus, the compromised concentration of y = 0.0025 was selected to produce a dual-emission from Pr^{3+} and Er^{3+}.

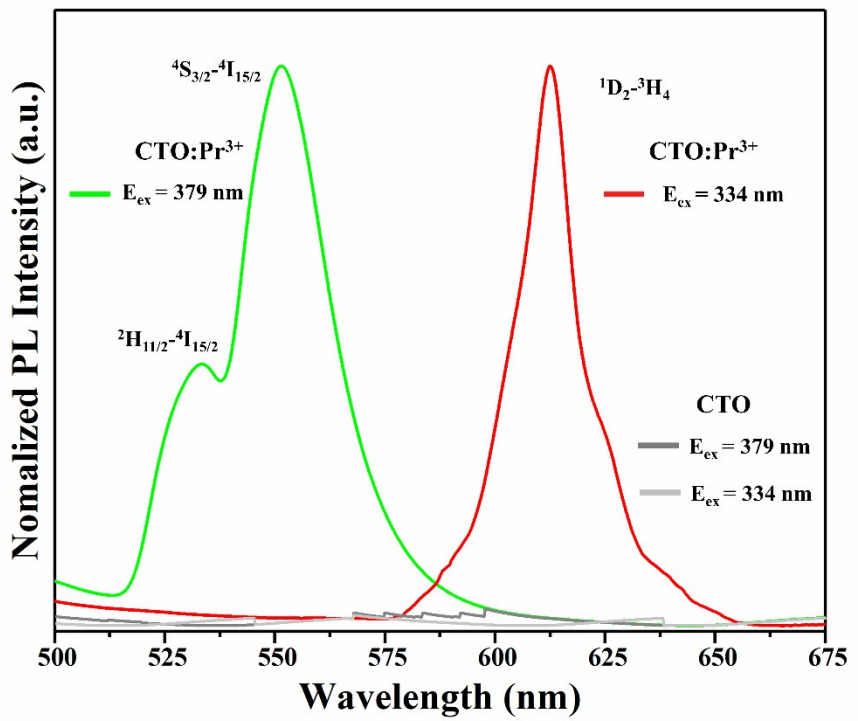

Fig. S6. PL spectra of CTO: R^{3+}(R^{3+} = Pr^{3+},Er^{3+}) and CTO samples.

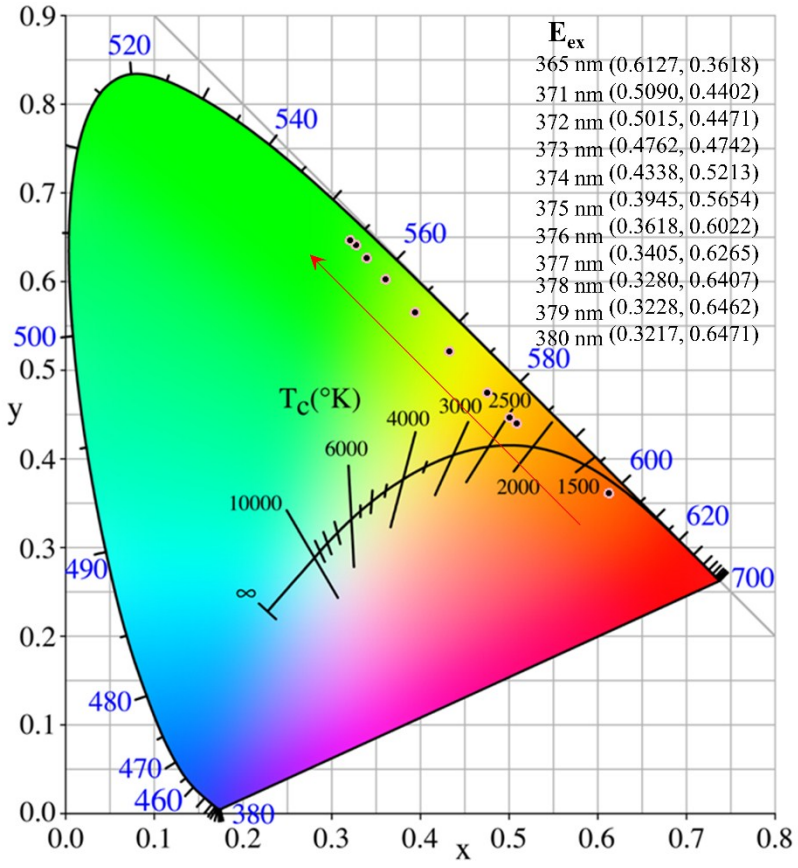

Fig. S7. CIE chromaticity diagram of the $CaTiO_3:Pr^{3+}$, Er^{3+} sample under different wavelengths irradiation.

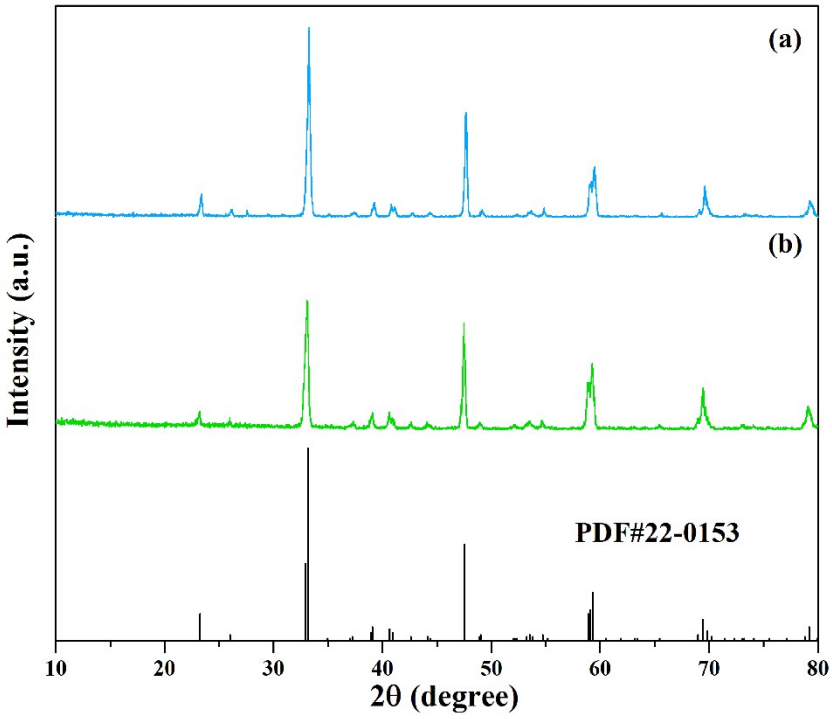

Fig. S8. (a) XRD pattern of the CTO:Pr^{3+},Er^{3+} after being heated with 1000℃. (b) XRD pattern of the CTO:Pr^{3+},Er^{3+} after being placed in tap water for 12 h

Table S1 (a). The refinement data for $CaTiO_3$.

Crystal data	
Chemical formula	$CaTiO_3$
Formula weight	260.96 g/mol
Crystalsystem	orthorhombic
Space group	P n m a (62)
Unit cell dimensions	a=5.3782(2)Å,b=5.4389(3)Å c=7.6380(1) Å
Volume	223.377(1) $Å^3$

Z	4
Density(calculated)	3.50354g/cm^3
X-ray diffractometer	Rigaku D/max-240
Temperature	298K
Theta range for data collection	10° to 80°
R_{wp}	14.0%
R_p	8.9%
χ^2	1.572

Table S1 (b). Atomic coordinates and isotropic displacement parameters for $CaTiO_3$.

Atom	Wyckoff	x/a	y/b	z/c	Fraction	U_{iso}
Ca_1	4c	-0.006	0.036	0.250	1	0.025
Ti_1	4b	0	0.5	0	1	0.025
O_1	4c	0.071	0.483	0.250	1	0.025
O_2	8d	0.710	0.288	0.037	1	0.025

Table S3. TL parameters of $CaTiO_3$:Pr^{3+}, Er^{3+}.

Trap	T_m(K)	E(eV)
1	344	0.69
2	383	0.77

The trap depths can be calculated by the Urbach method[3].

$$E = T_m/500$$

where Tm is the peak temperature (in Kelvin).

Notes and referencers

[1]. Dai, P. P.; Li, C.; Zhang, X. T.; Xu, J.; Chen, X.; Wang, X. L.; Liu, Y. C. A single Eu^{2+}-activated high-color-rendering oxychloride white-light phosphor for white-light-emitting diodes. *Light-Sci Appl*, **2016**, *5*, e16024-e16024.

[2]. Wang, J.; Lin, H.; Huang, Q.; Xiao, G.; Xu, J.; Wang, B; Wang, Y. Structure and luminescence behavior of a single-ion activated single-phased $Ba_2Y_3(SiO_4)_3F$: Eu white-light phosphor. *J. Mater. Chem. C*, **2017,** *5*, 1789-1797.

[3]. Hoerder, G. J.; Seibald, M.; Baumann, D.; Schröder, T.; Peschke, S.; Schmid, P. C.; Patzig, C. $Sr[Li_2Al_2O_2N_2]:Eu^{2+}$—A high performance red phosphor to brighten the future. *Nat. Commun*, **2019**, *10*, 1-9.