

SUPPORTING INFORMATION

CaSc₂O₄ Hosted Upconversion and Downshifting Luminescence

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Table S1 Typical Sc-based luminescent materials.

No.	Host material	Preparation method	Emission color	Size, morphology	Reference
1	$\text{Na}_x\text{ScF}_{3+x}:\text{Yb/Tm/Er}$ (18/0.2/x mol %)	Thermal coprecipitation	Green, red	27-36 nm nanoparticles	<i>J. Am. Chem. Soc.</i> , 2012, 134 , 8340-8343.
2	$\text{KSc}_2\text{F}_7:\text{Yb/Er}$	Thermal coprecipitation	red	376 nm nanorods	<i>Nanoscale</i> , 2013, 5 , 11928-11932
3	$\text{ScPO}_4 \cdot 2\text{H}_2\text{O}:\text{Ce,Tb}$	Hydrothermal	Green	2 μm micro-spheres	<i>J. Mater. Chem. C</i> , 2015, 3 , 12385-12389
4	$\text{Na}_x\text{ScF}_{3+x}:\text{Yb/Er}$	Thermal coprecipitation	From orange-red to green.	\sim 100 nm nanospheres and nanocubes	<i>Nanoscale</i> , 2015, 7 , 4048-4054
5	$\text{ScOOH}:\text{Eu}$, $\text{ScOOH}:\text{Tb}$	Hydrothermal	Red, green	1 μm microcrystals	<i>Adv. Mater.</i> , 2016, 26 , 6665-6671.
6	$\text{KSc}_2\text{F}_7:\text{Yb/Er}$	Thermal coprecipitation	Red	100 nm nanorods	<i>J. Mater. Chem. C</i> , 2017, 5 , 3503-3508
7	$\text{ScVO}_4:\text{Eu/Dy/Sm}$	Hydrothermal	Red, green, blue	10 μm microcrystals	<i>J. Rare Earth.</i> , 2017, 35 , 28-33.
8	$\text{KSc}_2\text{F}_7:\text{Yb/Er}$, $\text{K}_2\text{NaScF}_6:\text{Yb/Er}$	Thermal coprecipitation	Red	\sim 168.3 nm nanorods	<i>Dalton Trans.</i> , 2018, 47 , 4950-4958
9	$\text{Sc}_2\text{O}_3:\text{Eu}^{2+}/\text{Eu}^{3+}$	Thermal decomposition	Red, purple	\approx 20 nm nanoparticles	<i>Adv. Mater.</i> , 2018, 30 , 1705256.
10	$\text{ScF}_3:\text{Yb/Er}$, $\text{ScF}_{2.6}:\text{Yb/Er}$	Thermal coprecipitation	Green, yellow, blue	\approx 100 nm nanoparticles	<i>Chem. Mater.</i> , 2017, 29 , 9758-9766.

Table S2 Rietveld refinement of the crystallographic and structural parameters of CaSc₂O₄ and CaSc₂O₄:Yb/Tb (5/0.1 mol%).

Compounds	CaSc ₂ O ₄	CaSc ₂ O ₄ :Yb/Tb (5/0.1 mol%)
Crystal system	orthorhombic	orthorhombic
Lattice parameters	Pnam	Pnam
$\alpha = \beta = \gamma = 90^\circ$	a = 9.4555	a = 9.4747
(Å)	b = 11.1073	b = 11.1461
	c = 3.1404	c = 3.1537
V (Å)	V = 329.8211	V = 333.0457
Rwp(%)	9.7690	8.8500
Rp(%)	7.4100	6.7810
R _{exp}	9.0100	6.6500
χ^2	1.0830	1.3310

Table S3 Structural parameters and refinement data of CaSc₂O₄ and CaSc₂O₄:Yb/Tb (5/0.1 mol%).

Atom		CaSc ₂ O ₄	CaSc ₂ O ₄ : Yb/Tb (5/0.1 mol%)
Ca1	<i>x</i>	0.7536	0.7528
	<i>y</i>	0.6537	0.6552
	<i>z</i>	0.2500	0.2500
Sc1	<i>x</i>	0.4198	0.4247
	<i>y</i>	0.1071	0.1084
	<i>z</i>	0.2500	0.2500
Yb1	<i>x</i>	0.0000	0.4247
	<i>y</i>		0.1084
	<i>z</i>		0.2500
Tb1	<i>x</i>	00.0000	0.4247
	<i>y</i>		0.1084
	<i>z</i>		0.2500
Sc2	<i>x</i>	0.4279	0.4202
	<i>y</i>	0.6125	0.6132
	<i>z</i>	0.2500	0.2500
Yb2	<i>x</i>	0.0000	0.4202
	<i>y</i>		0.6132
	<i>z</i>		0.2500

Table S3 Structural parameters and refinement data of CaSc₂O₄ and CaSc₂O₄:Yb/Tb

(5/0.1 mol%). (Continued)

Tb2	<i>x</i>	0.0000	0.4202
	<i>y</i>		0.6132
	<i>z</i>		0.2500
O1	<i>x</i>	0.2045	0.1948
	<i>y</i>	0.1699	0.1670
	<i>z</i>	0.2500	0.2500
O2	<i>x</i>	0.1287	0.1252
	<i>y</i>	0.4752	0.4788
	<i>z</i>	0.2500	0.2500
O3	<i>x</i>	0.5233	0.5168
	<i>y</i>	0.7811	0.7891
	<i>z</i>	0.2500	0.2500
O4	<i>x</i>	0.4199	0.4100
	<i>y</i>	0.4233	0.4219
	<i>z</i>	0.2500	0.2500

Table S3 Structural parameters and refinement data of CaSc₂O₄ and CaSc₂O₄:Yb/Tb

(5/0.1 mol%). (Continued)

Bond lengths (Å)		
Sc1-O1	2.1520	2.2740
Sc1-O2	2.1760	2.1320
Sc1-O3	2.0730	2.1900
Sc2-O4	2.1670	2.1370
Sc1-Sc1	3.1404	3.1537
Sc2-Sc2	3.1404	3.1537
Yb1-Tb1		3.1537
Yb2-Tb2		3.1537
Bond angles (o)		
O2-Sc1-O2	91.2800	92.1300
O3-Sc1-O3	98.5100	102.3300
Sc1-O2-Sc1	91.2800	96.2300
Sc2-O1-Sc2	96.3700	103.410
Yb1-O2-Tb1		96.2300
Yb1-O3-Tb1		102.3300
Yb2-O4-Tb2		97.4900

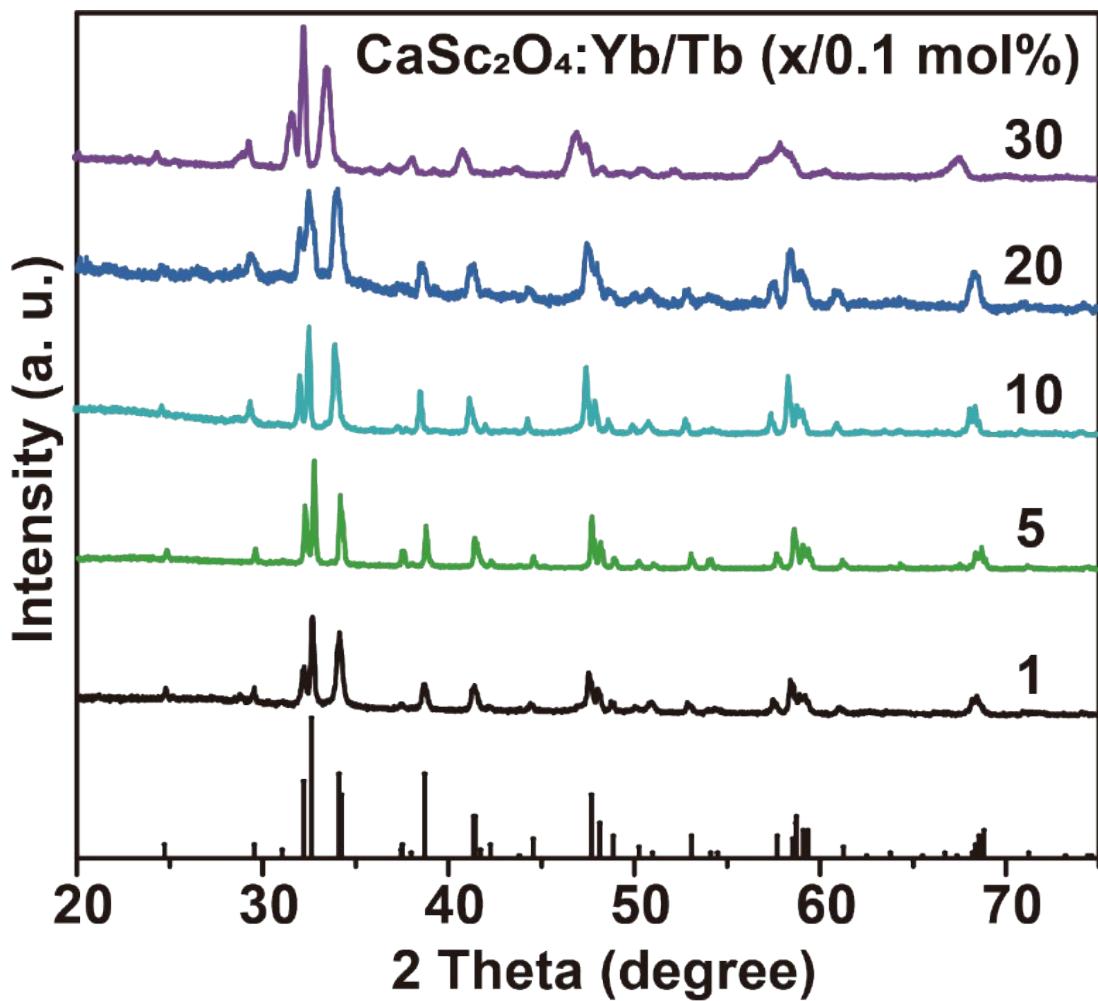


Fig. S1 XRD patterns of as-synthesized CaSc_2O_4 :Yb/Tb ($x/0.1 \text{ mol\%}$, $x = 1, 5, 10, 20, 30$) powders. The diffraction pattern at the bottom is the literature reference of orthorhombic CaSc_2O_4 crystal (JCPDS: 20-0234).

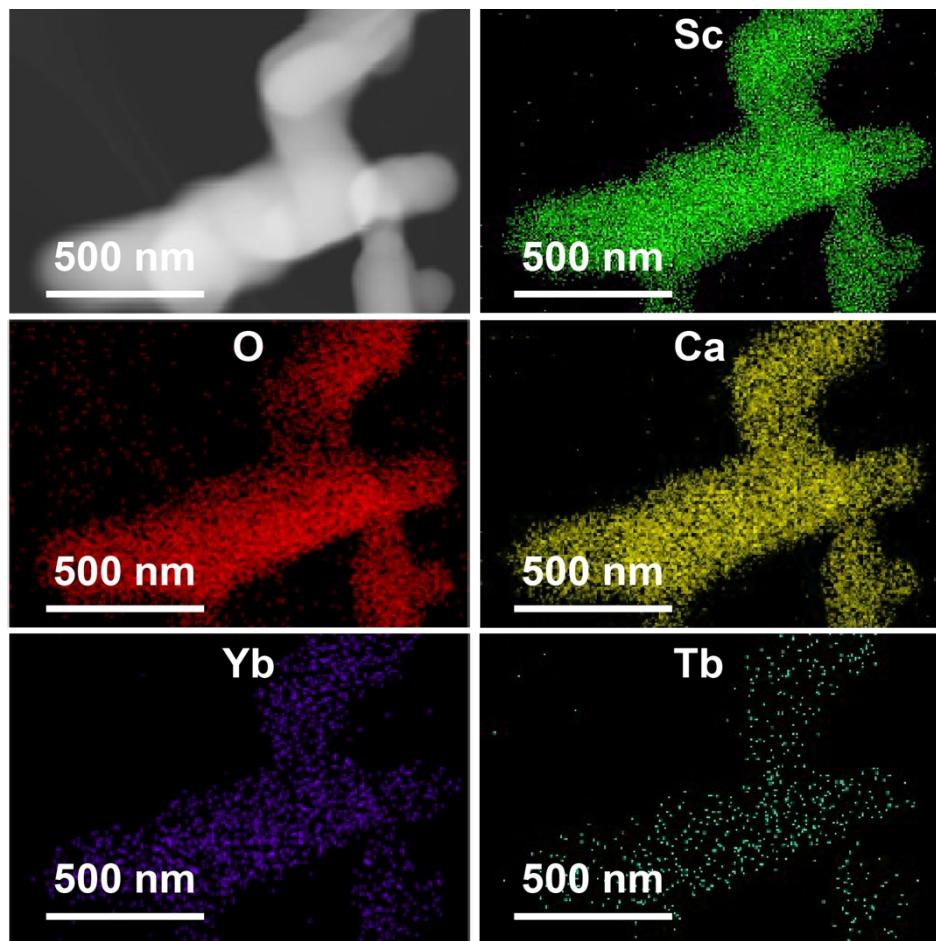


Fig. S2 EDX mapping results of CaSc_2O_4 :Yb/Tb (5/0.1 mol%) powder.

Table S4 Elemental analysis of CaSc₂O₄: Yb/Ln (Ln = Tb³⁺ or Eu³⁺)

No.	Materials	Yb/Ln Doped (mol%)	Yb/Ln Detected (mol%)
1	CaSc ₂ O ₄ :Yb/Tb	Yb/Tb (5/0.1)	Yb/Tb (3.6/0.07)
2	CaSc ₂ O ₄ :Yb/Eu	Yb/Eu (5/2)	Yb/Eu (2.01/0.02)

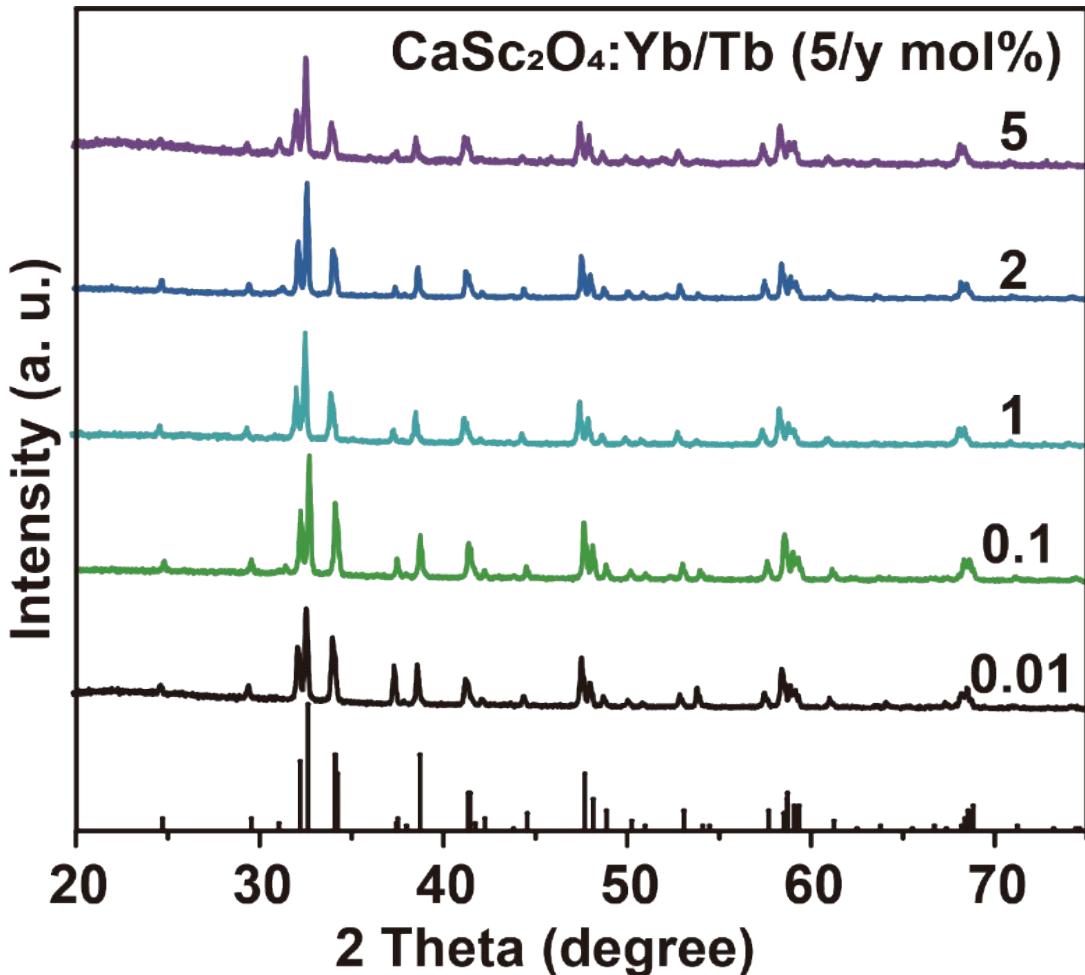


Fig. S3 XRD patterns of as-synthesized CaSc₂O₄:Yb/Tb (5/y mol%, y = 0.01, 0.1, 1, 2, 5) powders. The diffraction pattern at the bottom is the literature reference of orthorhombic CaSc₂O₄ crystal (JCPDS: 20-0234).

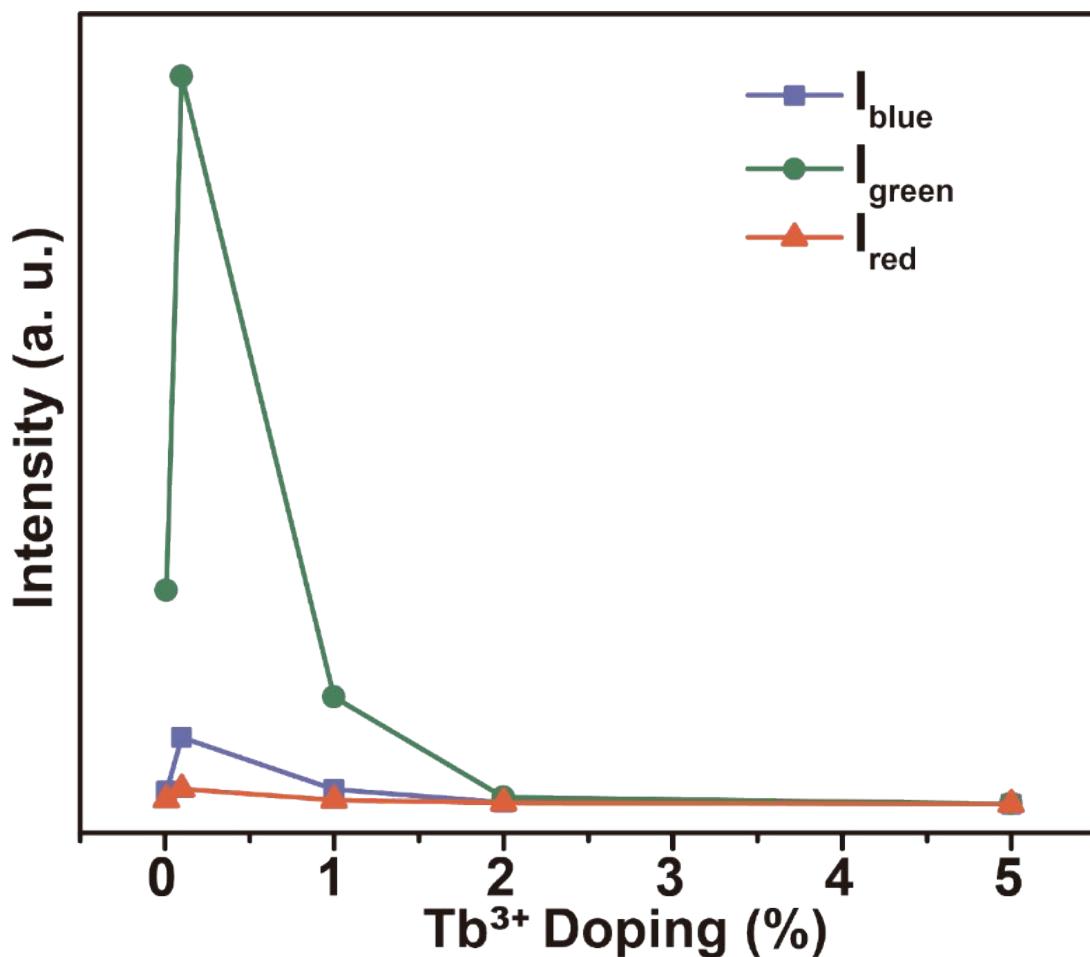


Fig. S4 The dependence of UCL emission intensity on Tb^{3+} doping concentration in $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ ($5/\text{y}$ mol%, $\text{y} = 0.01, 0.1, 1, 2, 5$).

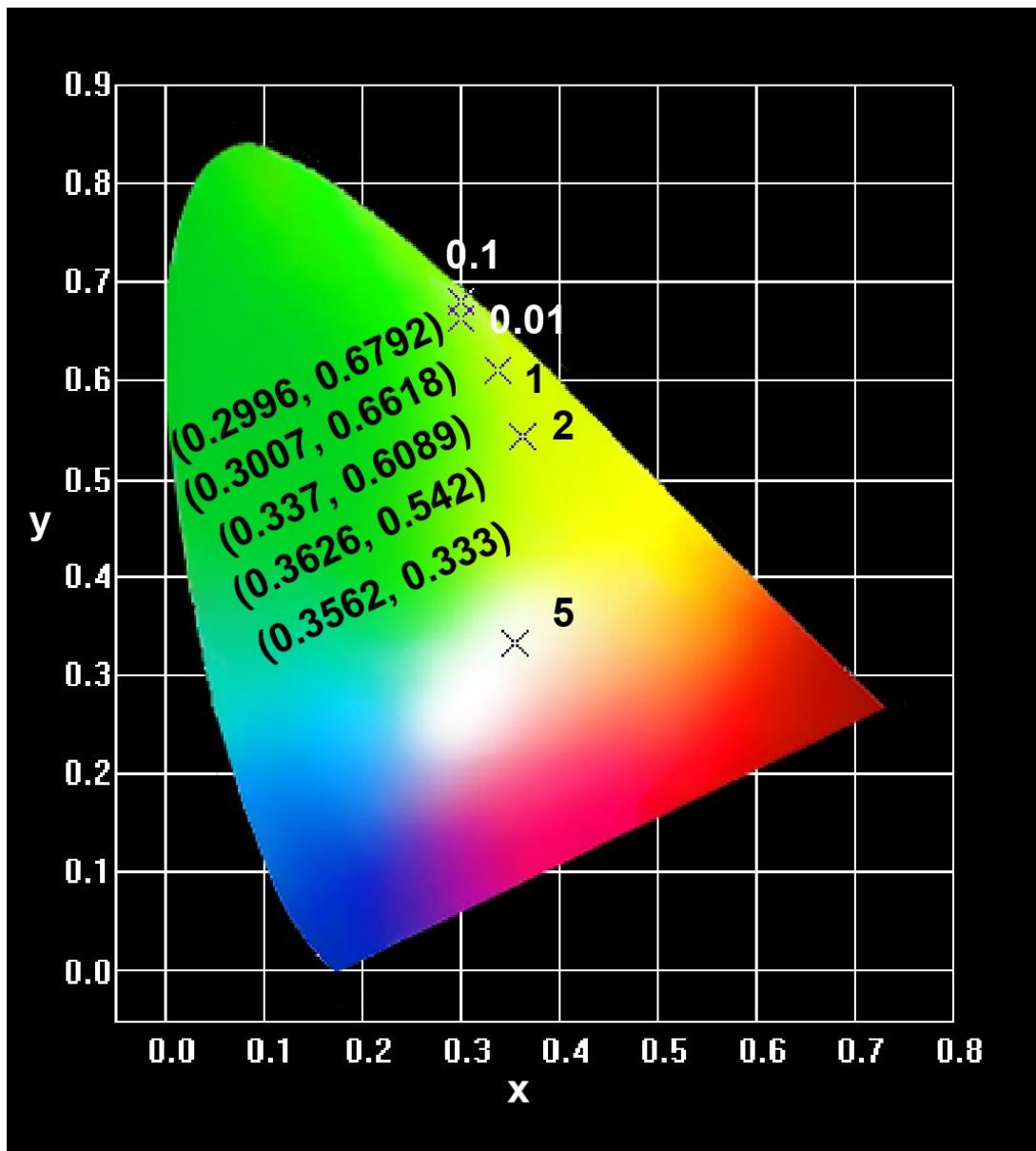


Fig. S5 The CIE color coordinates of CaSc₂O₄:Yb/Tb (5/y mol%, y = 0.01, 0.1, 1, 2, 5) powders.

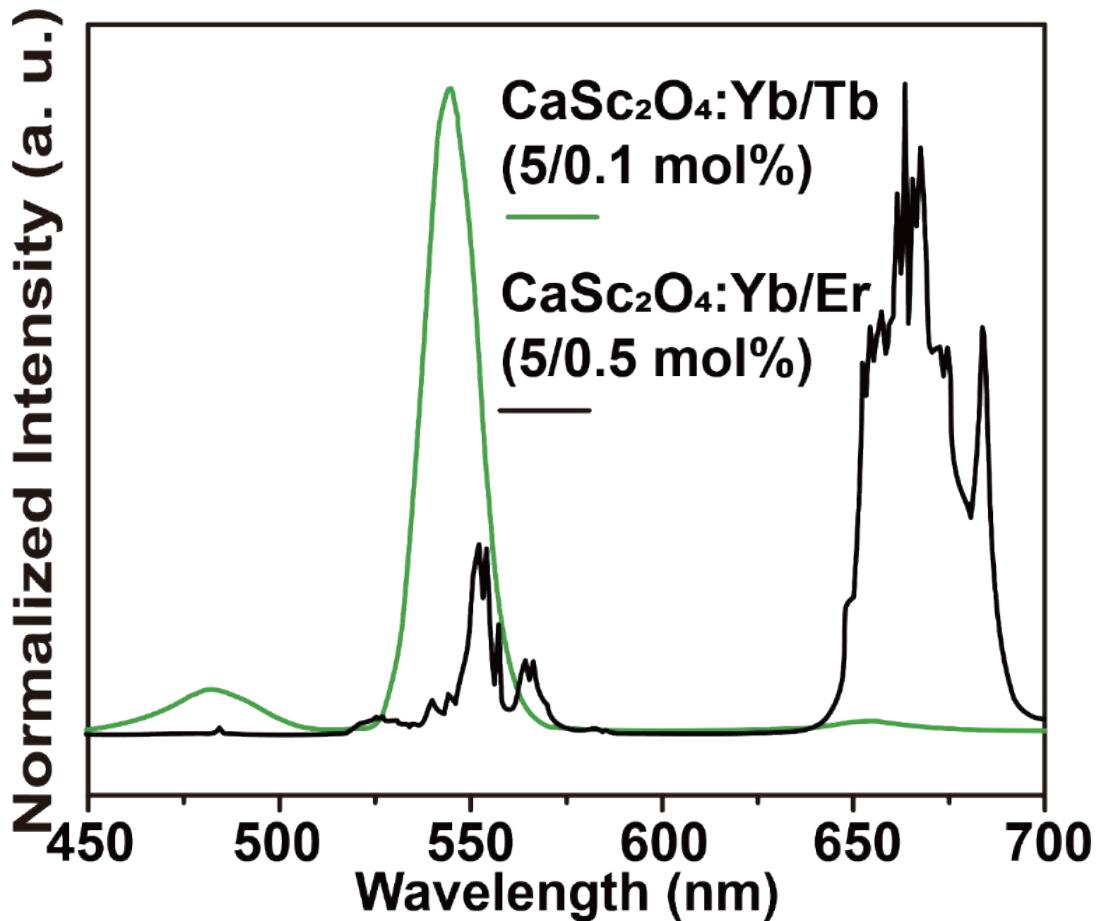


Fig. S6 Normalized intensity of UCL spectra of $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ (5/0.1 mol%) and $\text{CaSc}_2\text{O}_4:\text{Yb/Er}$ (5/0.5 mol%) powders under the excitation of a 980 nm laser.

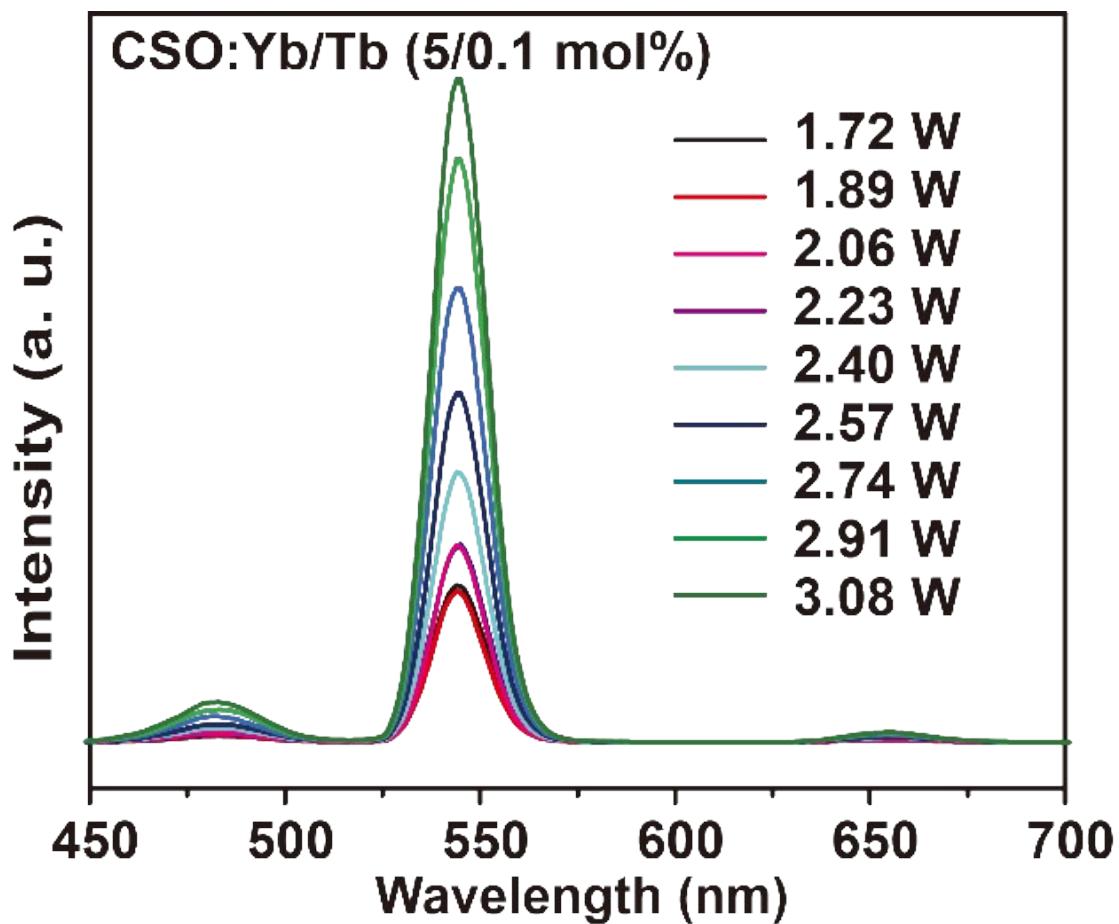


Fig. S7 UCL spectra of CaSc₂O₄:Yb/Tb (5/0.1 mol%) powders at different excitation powers of a 980 nm laser.

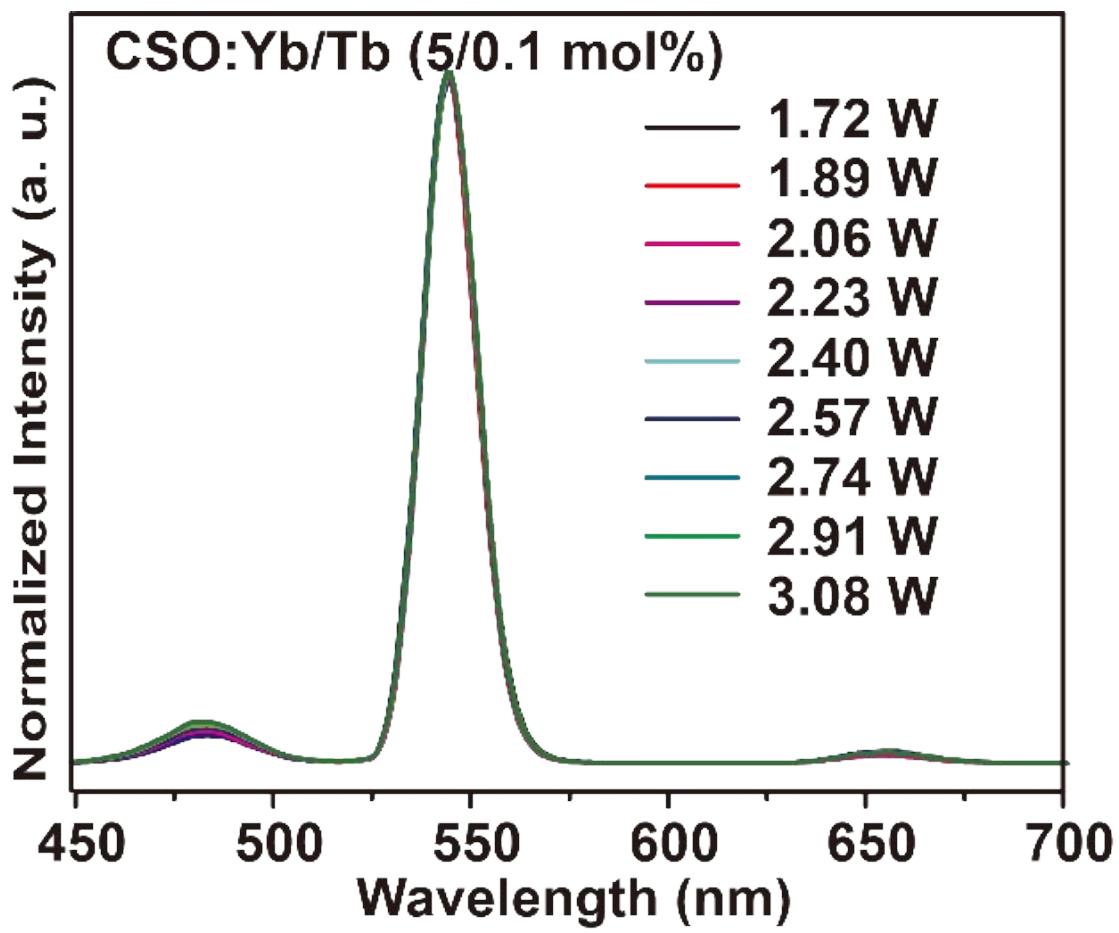


Fig. S8 Normalized intensity of UCL spectra of CaSc₂O₄:Yb/Tb (5/0.1 mol%) powders at different excitation powers of a 980 nm laser.

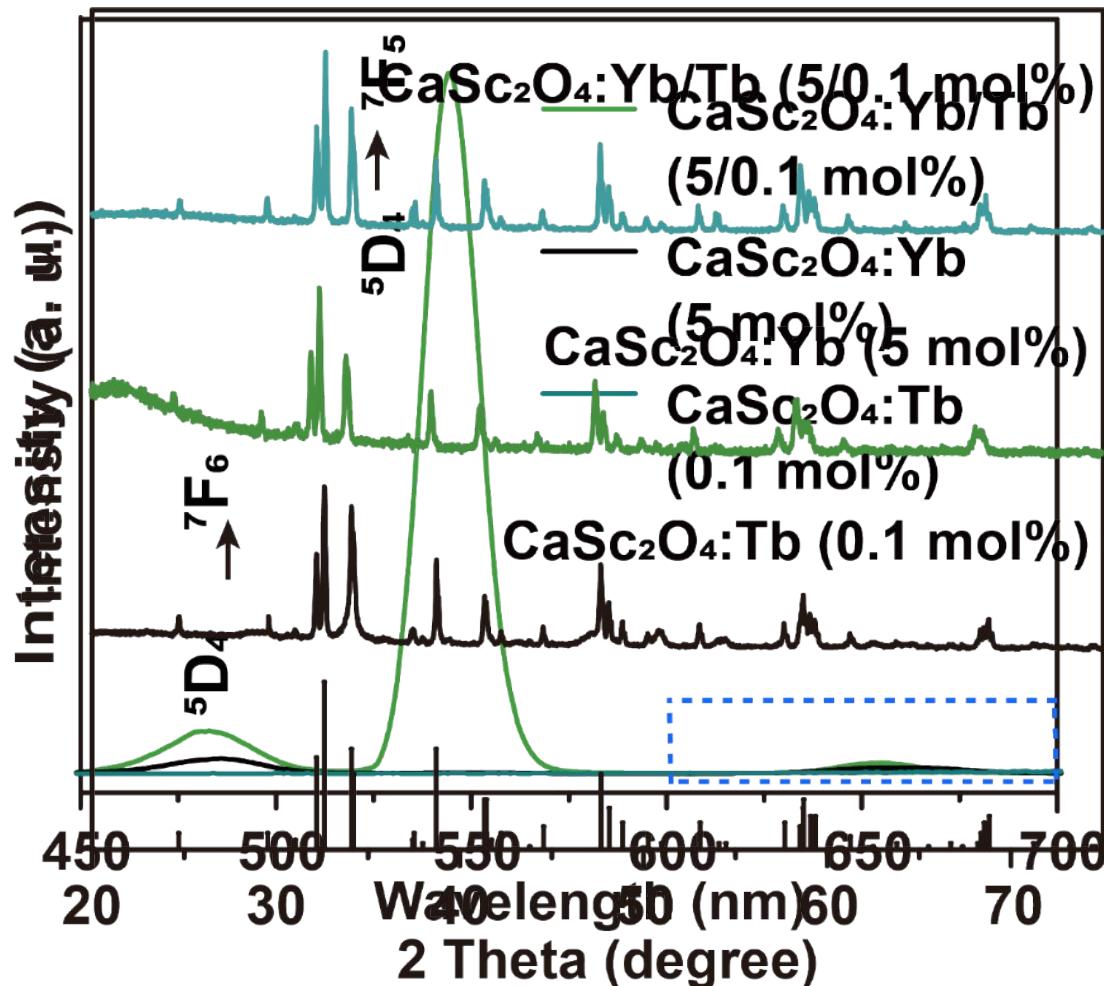


Fig. S9 XRD patterns of the as-synthesized $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ (5/0.1 mol%), $\text{CaSc}_2\text{O}_4:\text{Yb}$ (5 mol%), and $\text{CaSc}_2\text{O}_4:\text{Tb}$ (0.1 mol%) powders. The diffraction pattern at the bottom is the reference of orthorhombic CaSc_2O_4 crystal (JCPDS: 20-0234).

Fig. S10 UCL spectra of $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ (5/0.1 mol%), $\text{CaSc}_2\text{O}_4:\text{Yb}$ (5 mol%) and $\text{CaSc}_2\text{O}_4:\text{Tb}$ (0.1 mol%) powders under the excitation of a 980 nm laser.

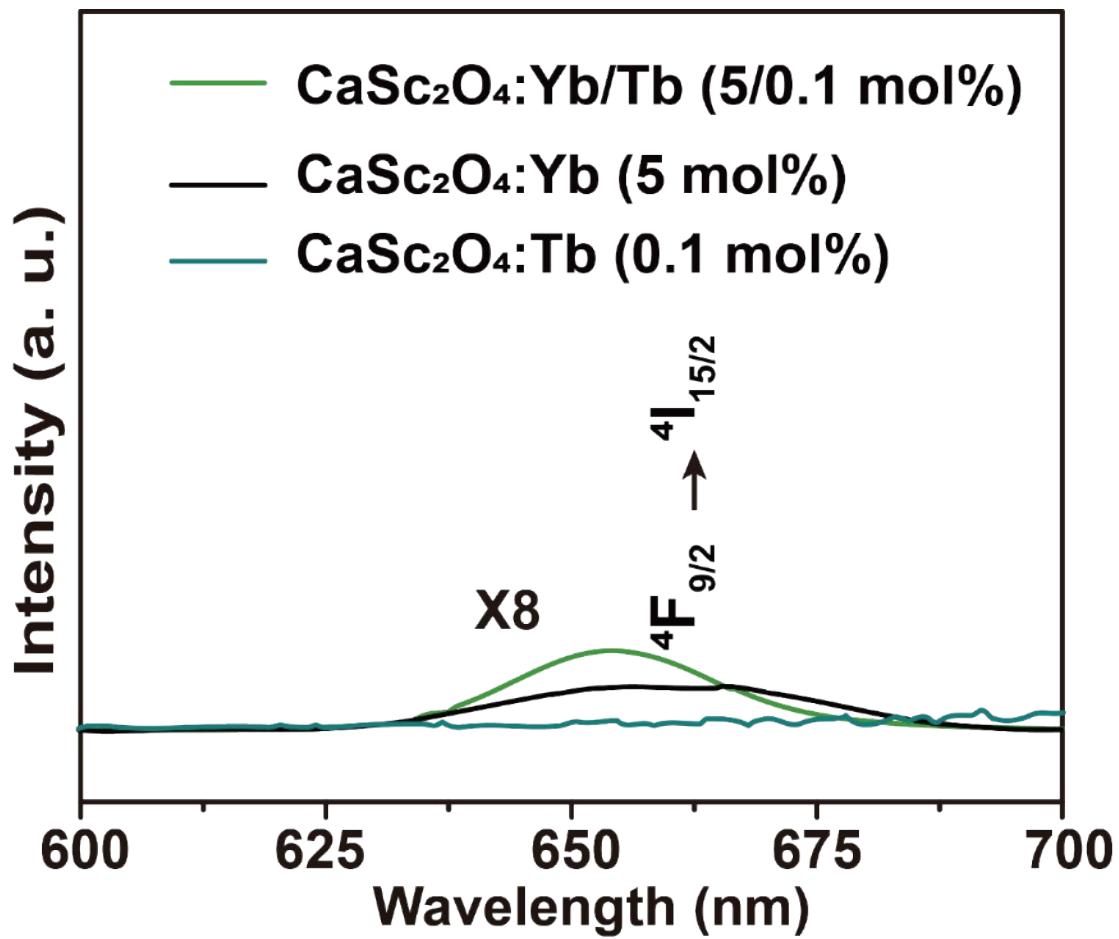


Fig. S11 The enlarged UCL spectra of $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ (5/0.1 mol%), $\text{CaSc}_2\text{O}_4:\text{Yb}$ (5 mol%) and $\text{CaSc}_2\text{O}_4:\text{Tb}$ (0.1 mol%) powders in the region of 600-700 nm under the excitation of a 980 nm laser.

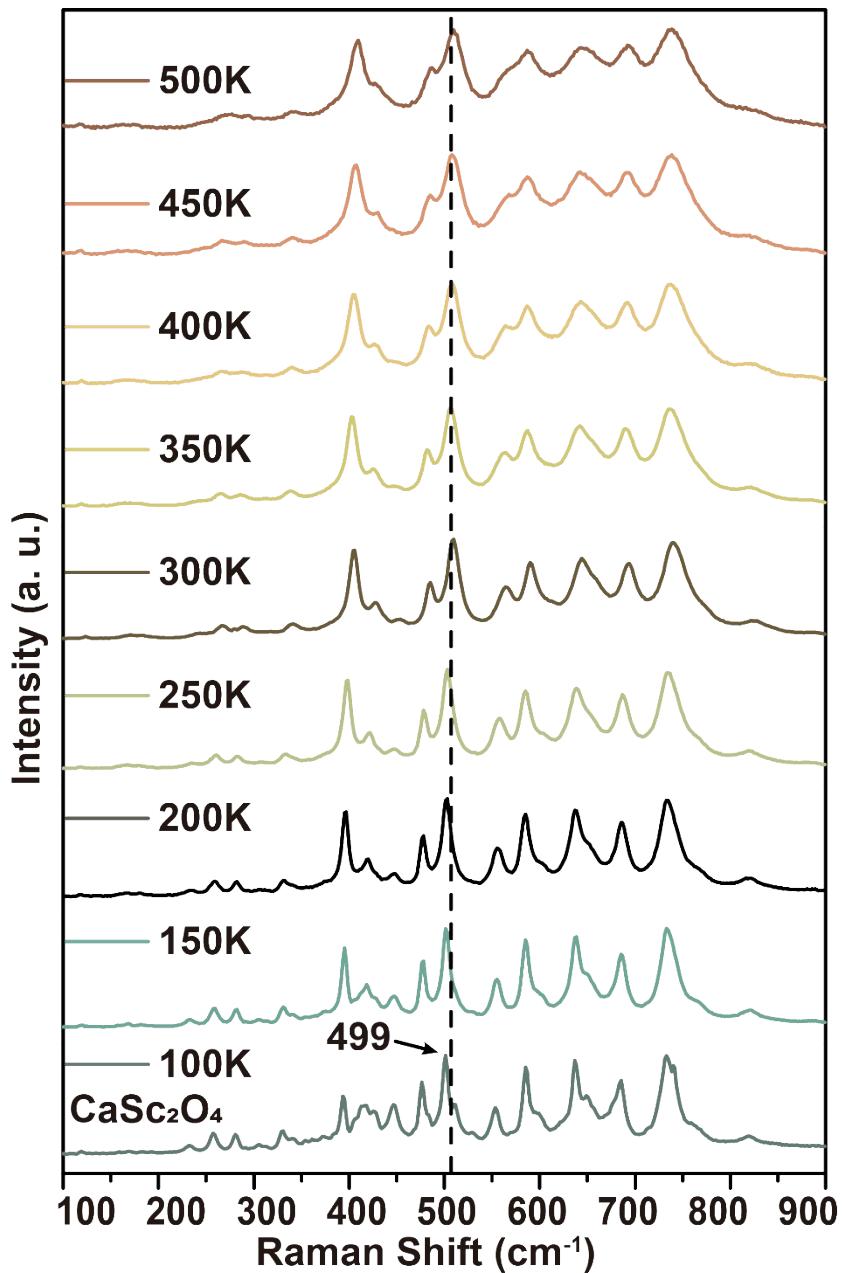


Fig. S12 Temperature-dependent Raman spectra of CaSc_2O_4 at temperature range of 100–500 K.

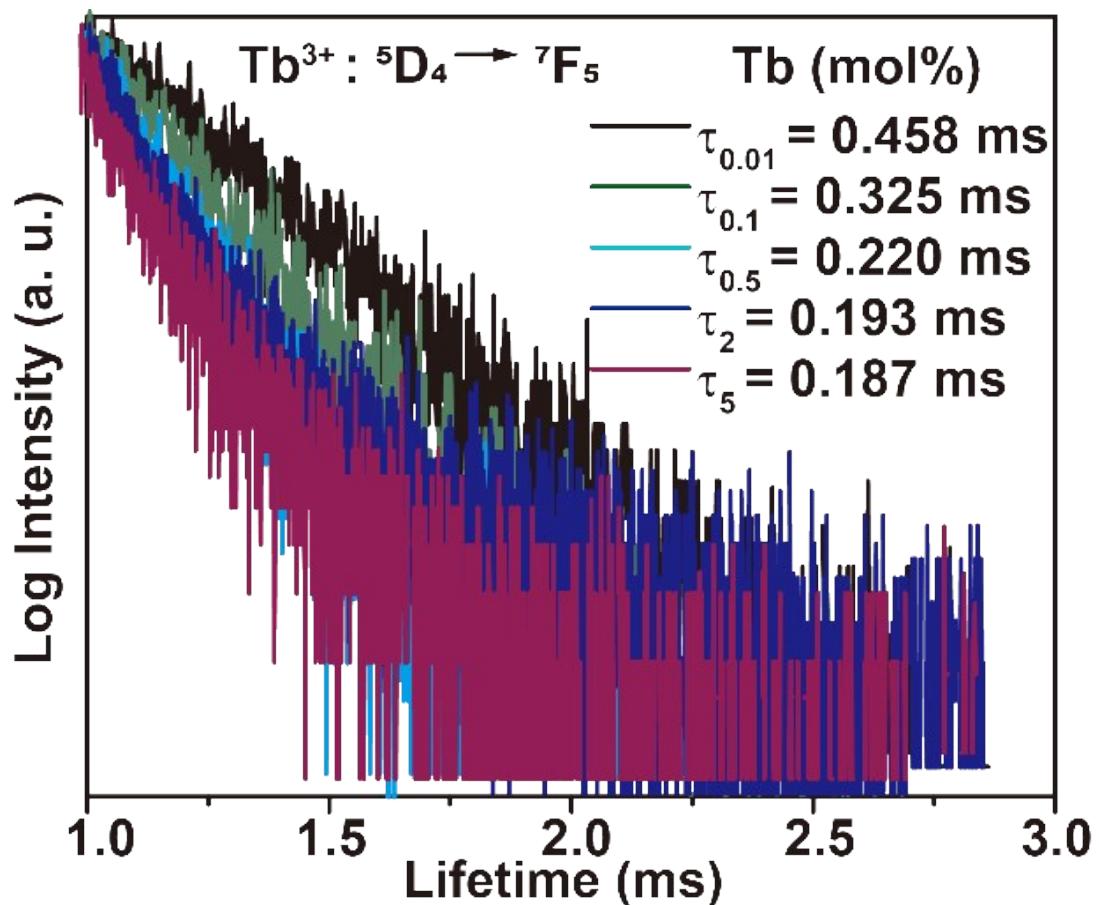


Fig. S13 UCL decay curves of ${}^5\text{D}_4 \rightarrow {}^7\text{F}_5$ transition of Tb^{3+} in $\text{CaSc}_2\text{O}_4:\text{Yb/Tb}$ ($5/\text{y}$ mol%, $\text{y} = 0.01, 0.1, 1, 2, 5$) powders excited under a 980 nm pulsed laser.

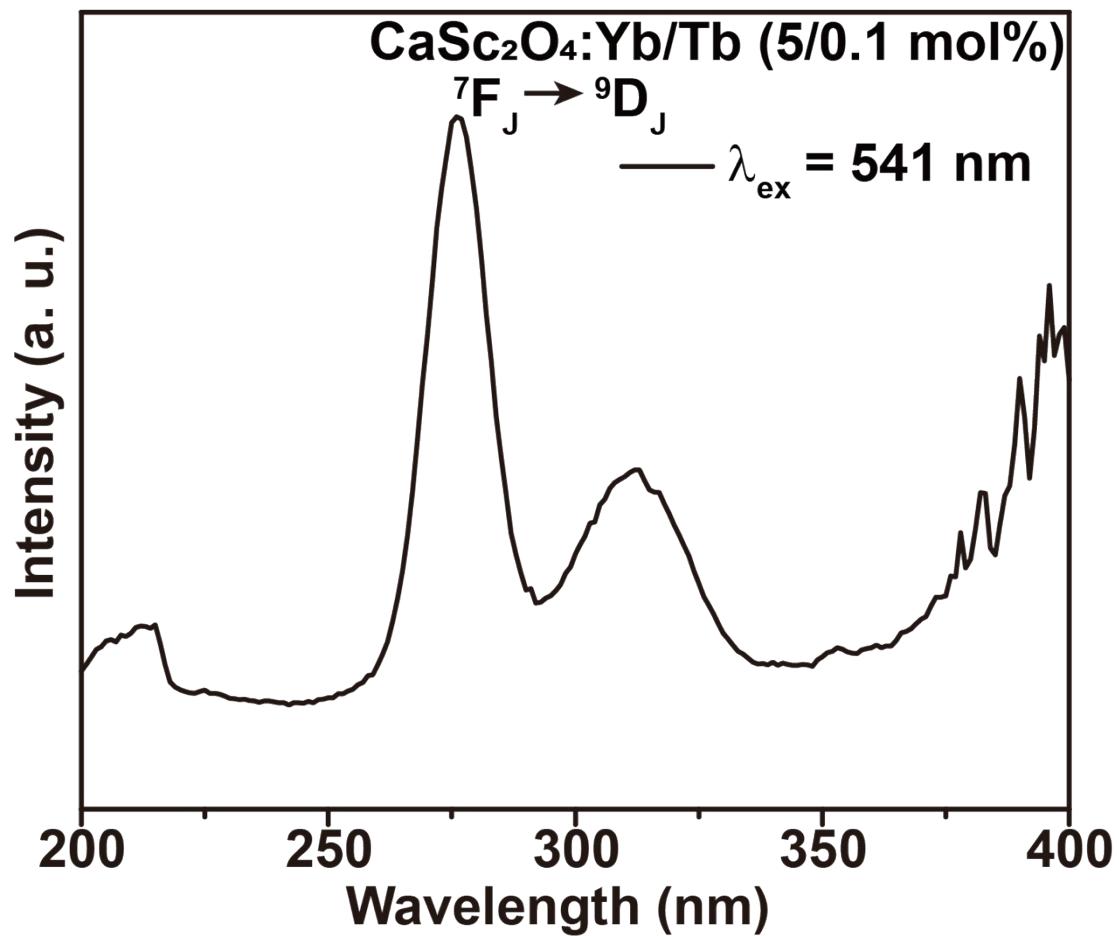


Fig. S14 Photoluminescence excitation spectrum of CaSc₂O₄:Yb/Tb (5/0.1 mol%) monitored at emission of 541 nm.

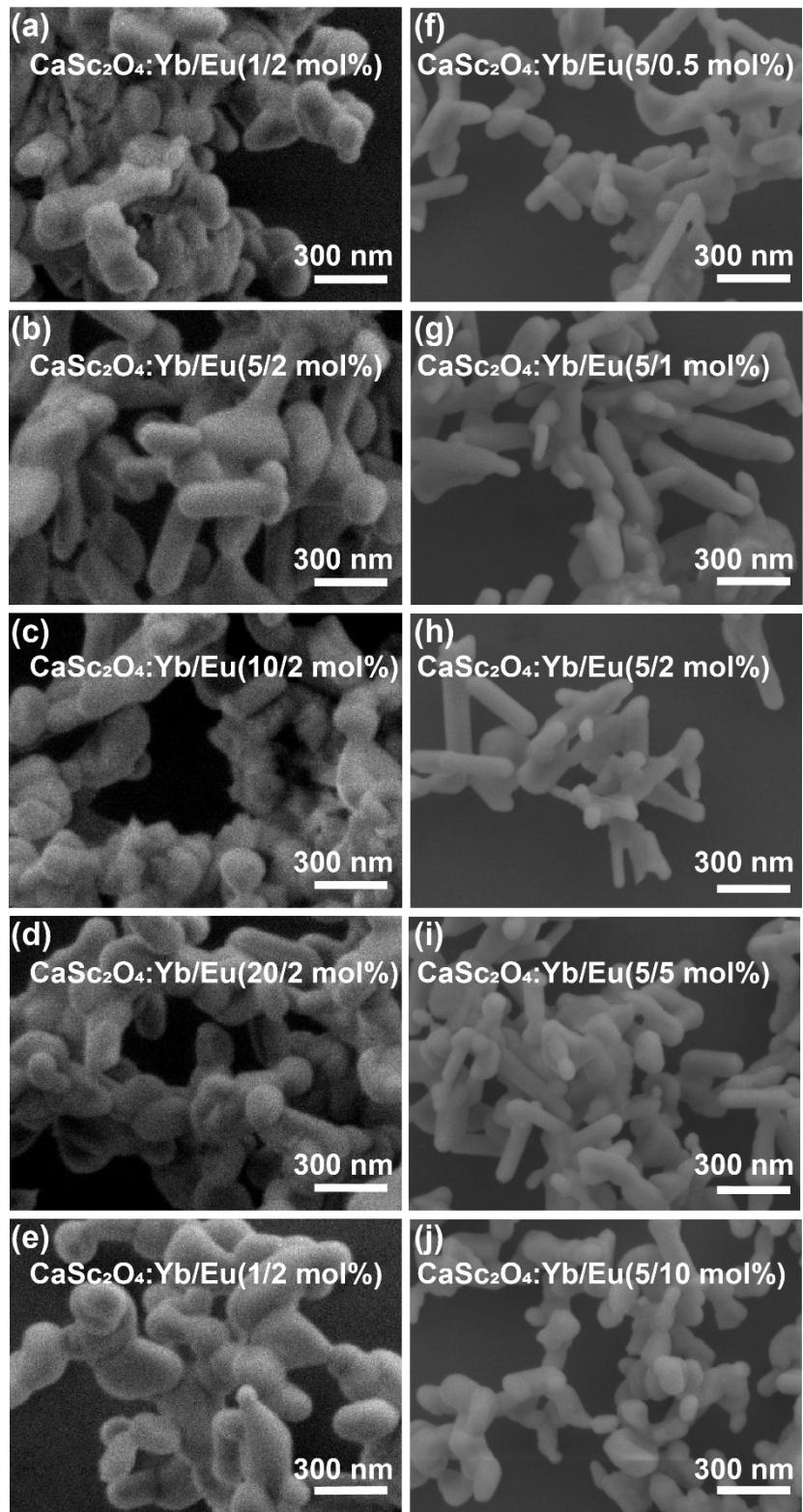


Fig. S15 SEM images of (a-e) as-synthesized $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ ($x/2 \text{ mol}\%$, $x = 1, 5, 10, 20, 30$) powders, (f-j) $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ ($5/y \text{ mol}\%$, $y = 0.5, 1, 2, 5, 10$) powders.

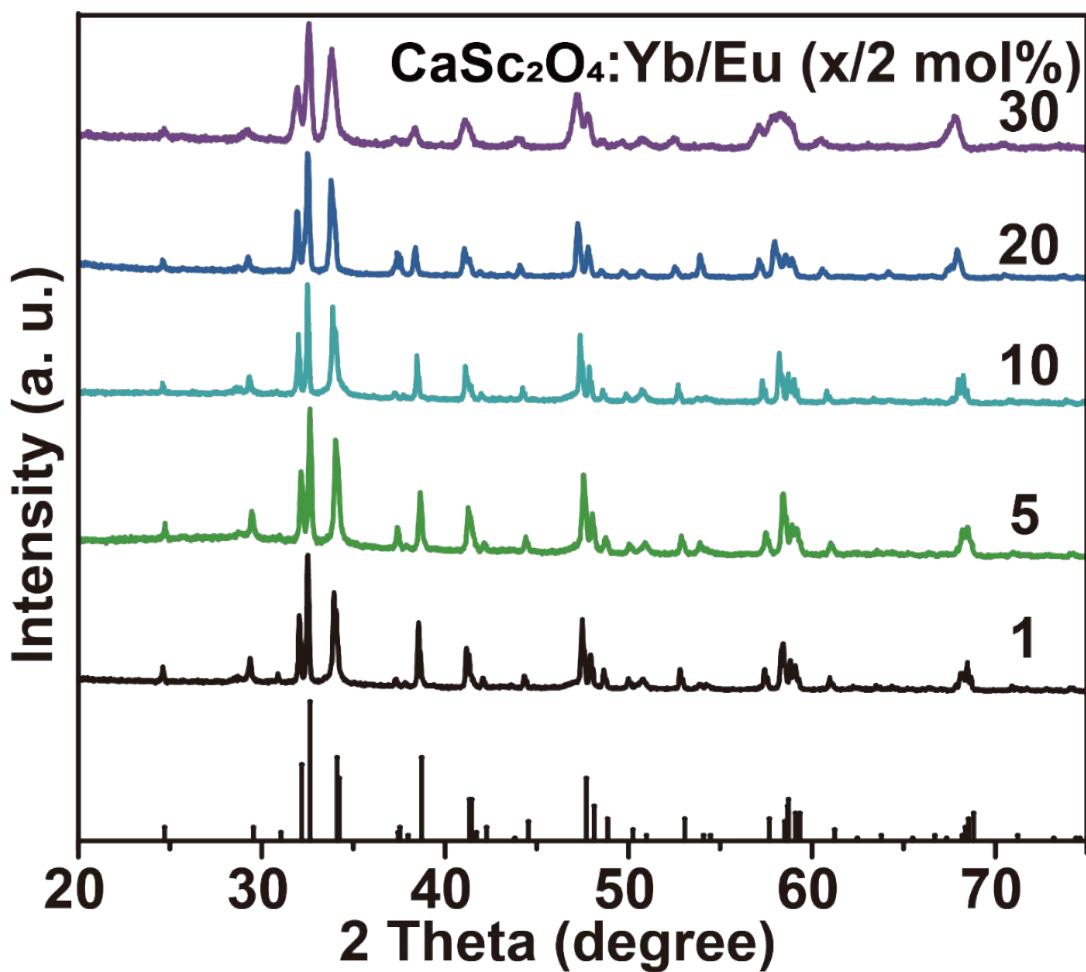


Fig. S16 XRD patterns of as-synthesized CaSc_2O_4 :Yb/Eu ($x/2 \text{ mol\%}$, $x = 1, 5, 10, 20, 30$) powders. The diffraction pattern at the bottom is the literature reference of orthorhombic CaSc_2O_4 crystal (JCPDS: 20-0234).

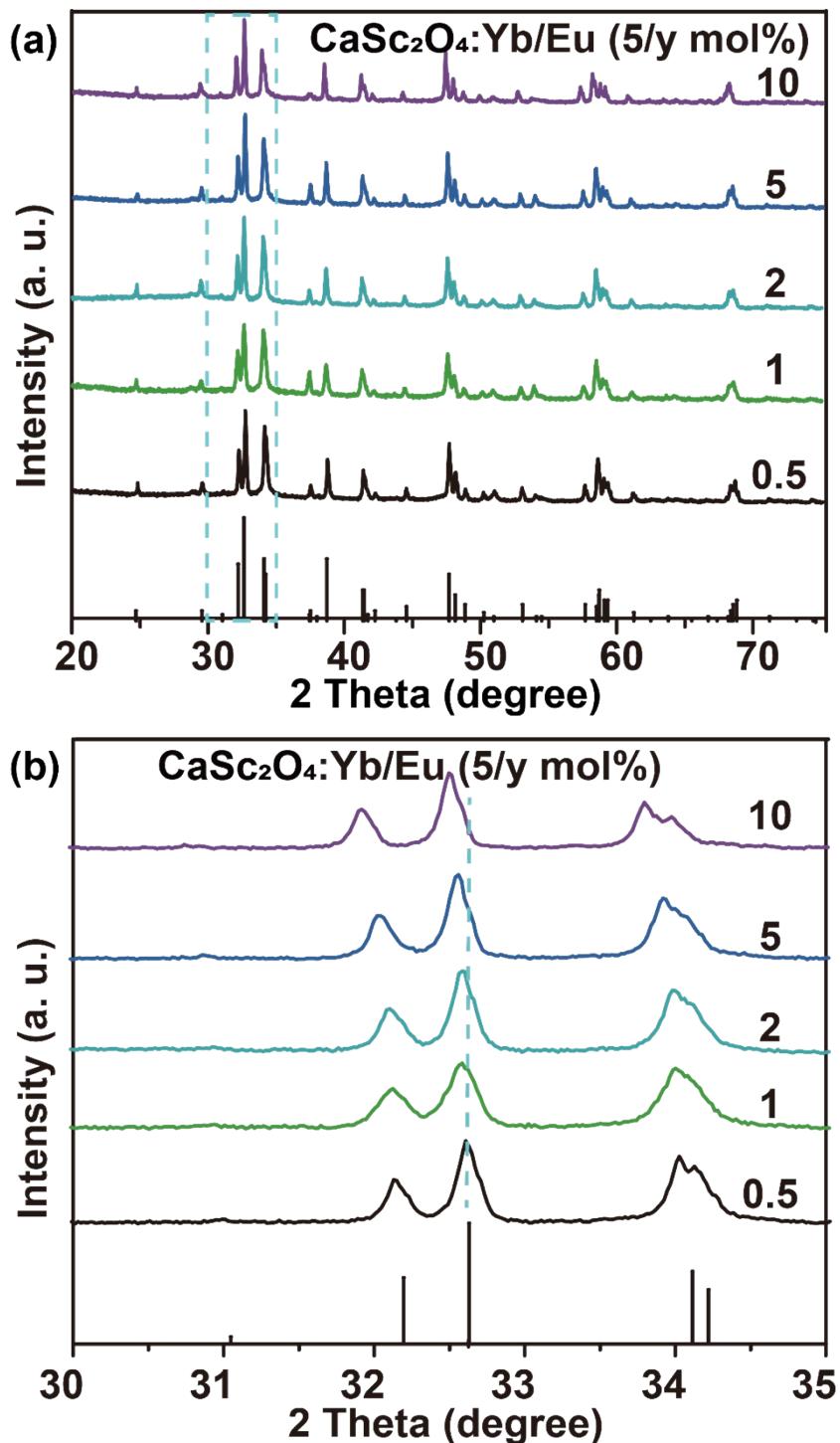


Fig. S17 (a) XRD and (b) enlarged XRD patterns of $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ (5/y mol%, $y = 0.5, 1, 2, 5, 10$) powders. The diffraction pattern at the bottom is the literature reference of orthorhombic CaSc_2O_4 crystal (JCPDS: 20-0234).

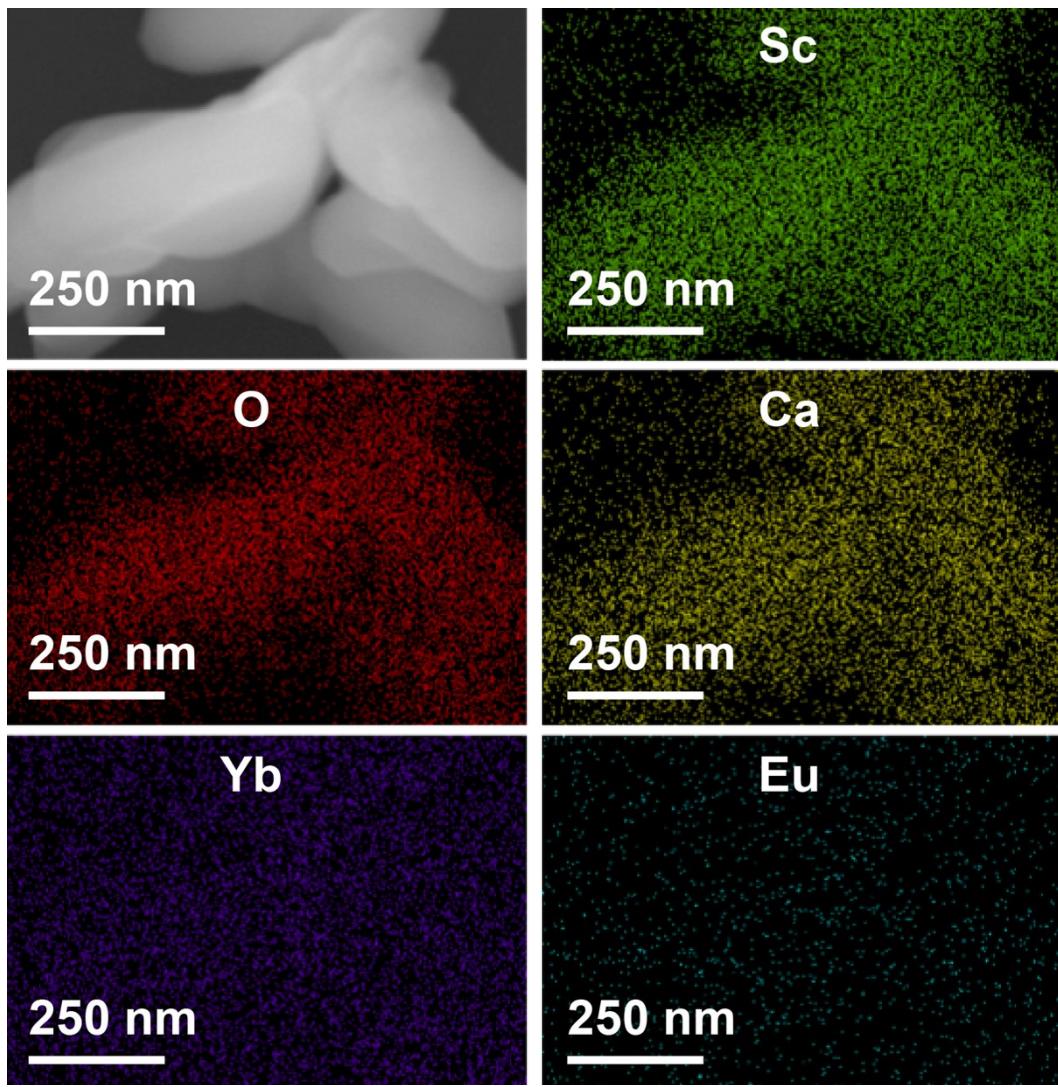


Fig. S18 EDX mapping results of CaSc_2O_4 : Yb/Eu (5/2 mol%) powder.

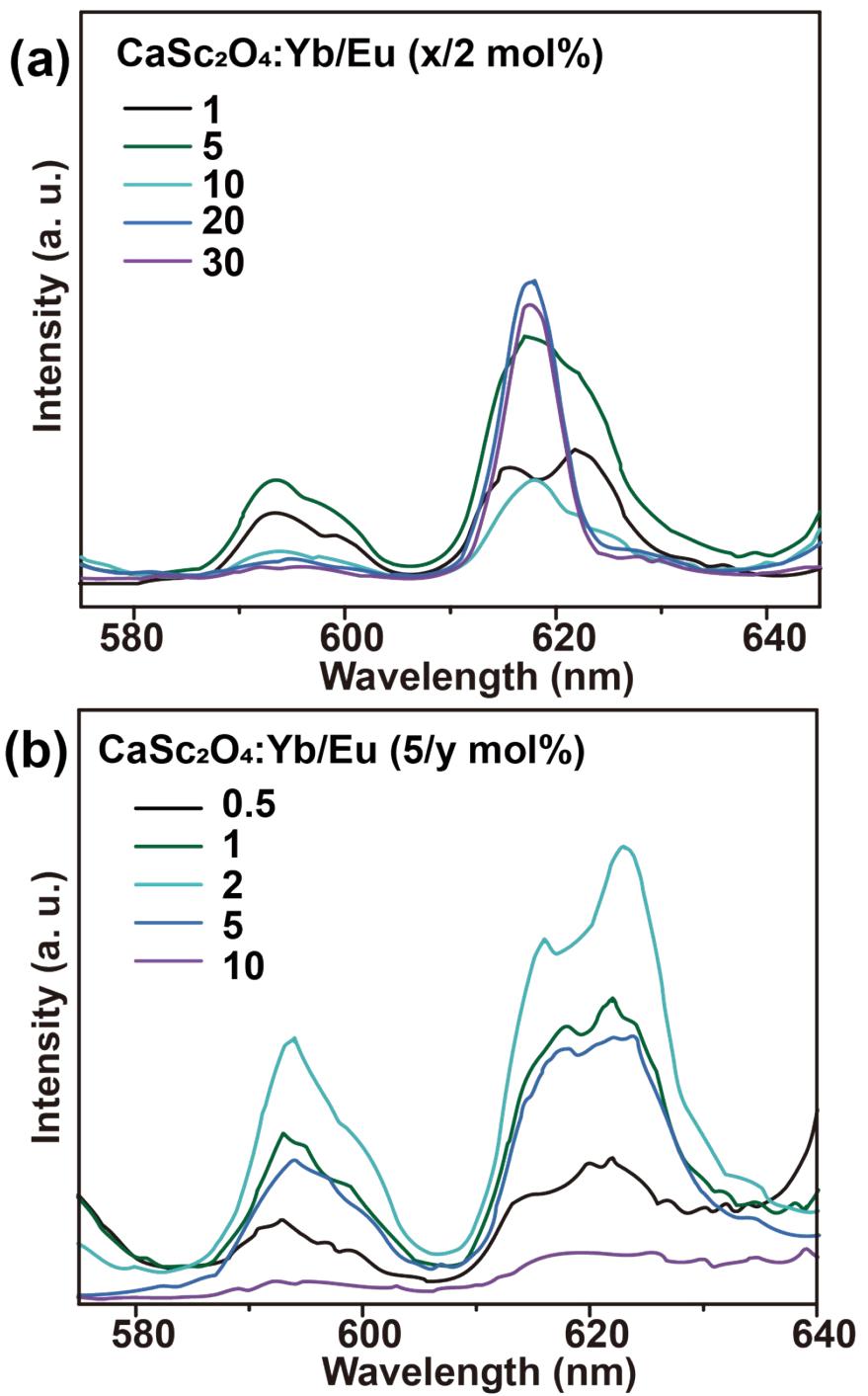


Fig. S19 (a) UCL spectra of $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ ($x/2 \text{ mol\%}$, $x = 1, 5, 10, 20, 30$) powders and (b) $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ ($5/y \text{ mol\%}$, $y = 0.5, 1, 2, 5, 10$) powders under the excitation of a 980 nm laser.

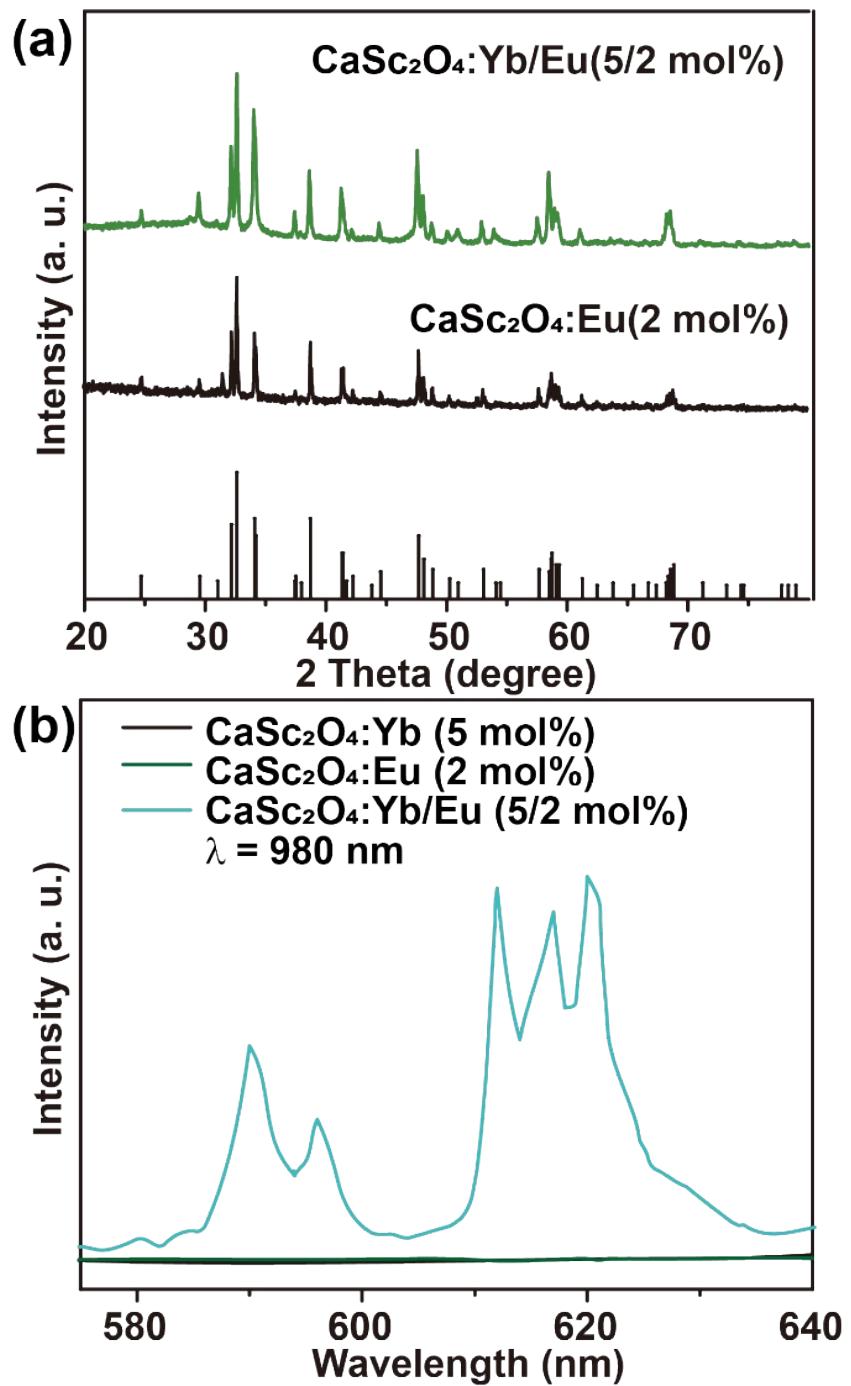


Fig. S20 (a) XRD patterns of as-synthesized CaSc₂O₄:Yb/Eu (5/2 mol%) and CaSc₂O₄:Eu (2 mol%) powders. The diffraction pattern at the bottom is the literature reference of orthorhombic CaSc₂O₄ crystal (JCPDS: 20-0234). (b) UCL spectra of CaSc₂O₄:Yb (5 mol%), CaSc₂O₄:Eu (2 mol%), and CaSc₂O₄:Yb/Eu (5/2 mol%) powders under the excitation of a 980 nm laser.

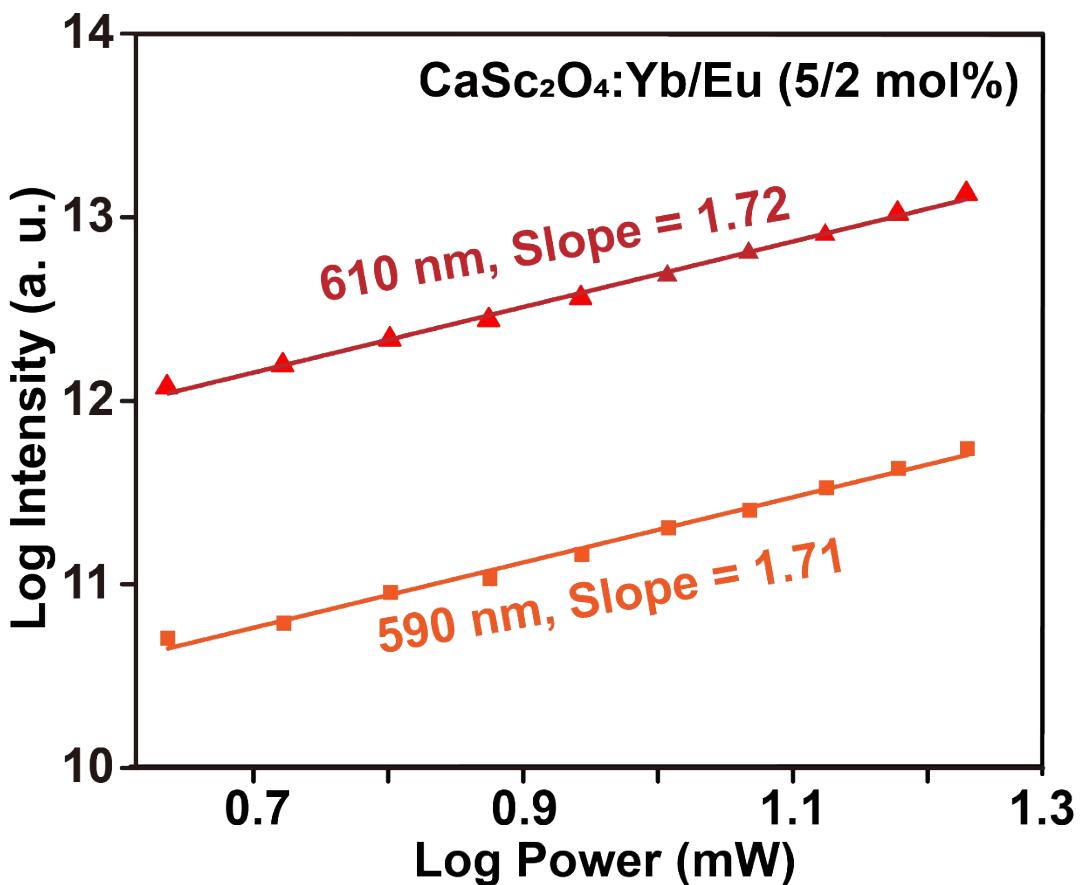


Fig. S21 Log-log plots of the upconversion emission intensities at 590 and 610 nm of CaSc₂O₄:Yb/Eu (5/2 mol%) powders versus excitation power of the 980 nm laser.

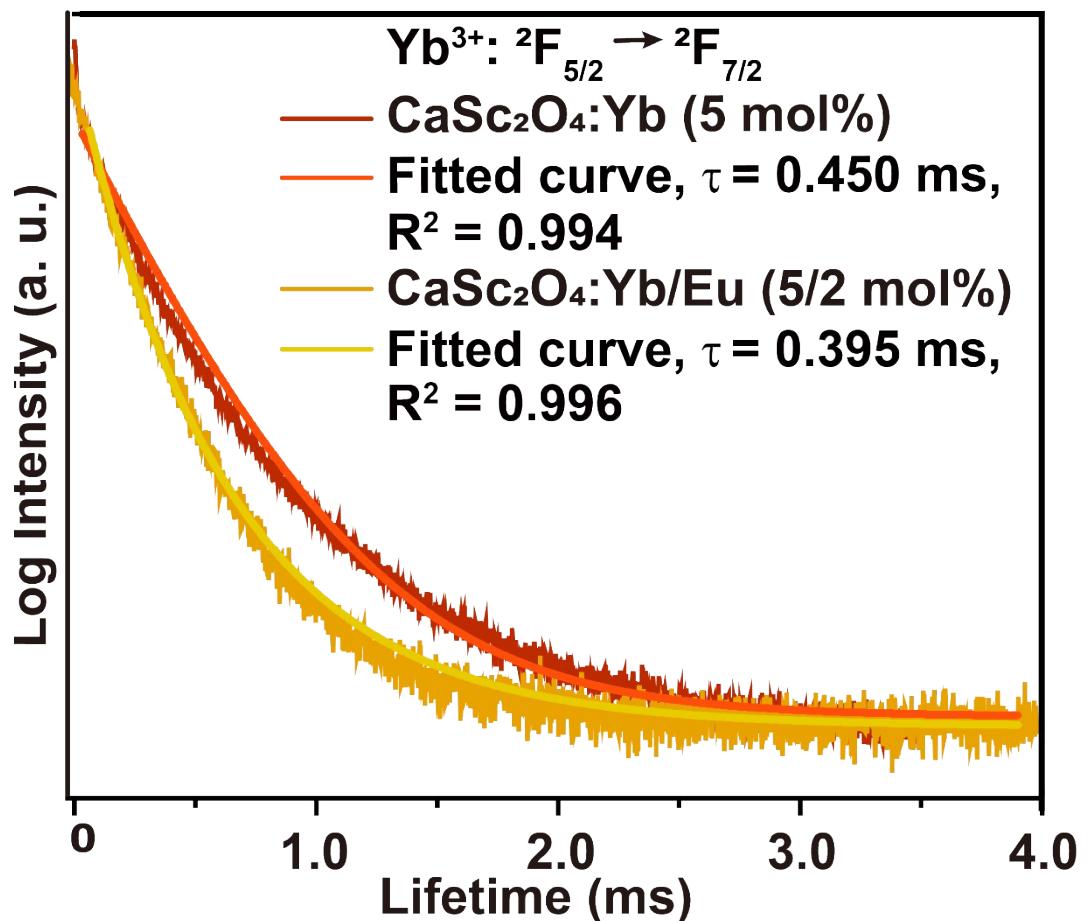


Fig. S22 Luminescence decay curves of $^2F_{5/2} \rightarrow ^2F_{7/2}$ transition of Yb³⁺ in CaSc₂O₄:Yb (5 mol%) and CaSc₂O₄:Yb/Eu (5/2 mol%) powders, respectively, excited under a 980 nm pulsed laser.

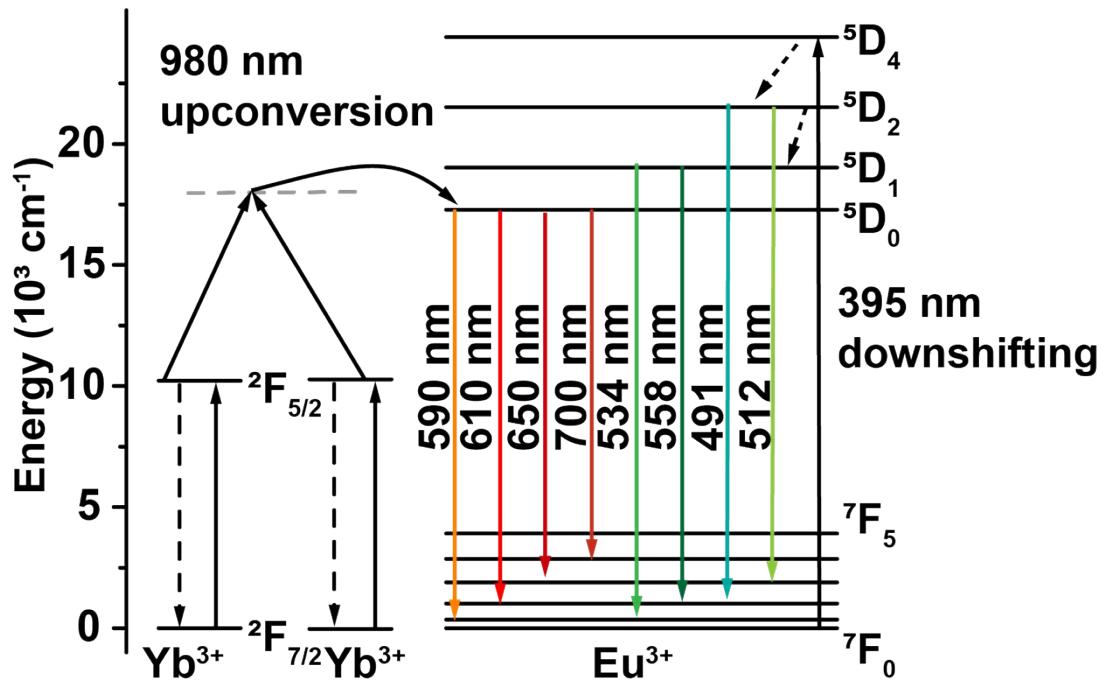


Fig. S23 Schematic illustration of the upconversion and downshifting luminescence mechanism in $\text{CaSc}_2\text{O}_4:\text{Yb}/\text{Eu}$ under excitation of a 980 and 395 nm light, respectively.

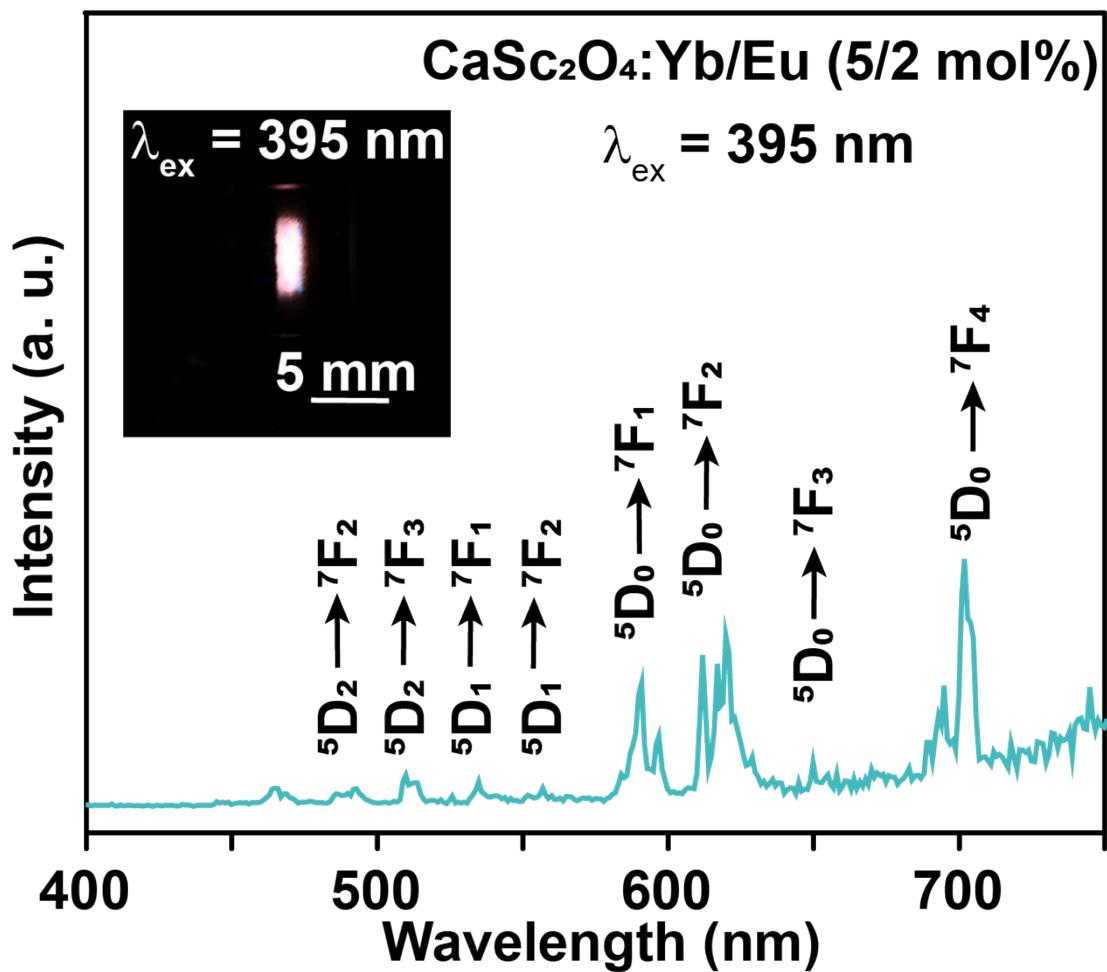


Fig. S24 Downshifting luminescence spectrum of CaSc₂O₄:Yb/Eu (5/2 mol%) excited by a 395 nm light. The inset is the photograph of CaSc₂O₄:Yb/Eu (5/2 mol%) powders under the excitation of a 395 nm.