Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information for:

Simultaneous Enhancement of Near Infrared Luminescence and Stability of $Cs_2AgInCl_6:Cr^{3+}$ Double Perovskites Single Crystal Enabled by Yb^{3+} Dopant

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Experimental

1. Materials

The following chemicals were used as purchased without further purification: CsCl (99%, Aladdin), AgCl (99.5, Macklin), $InCl_3$ (99.99%, Aladdin), $CrCl_3 \cdot 6H_2O$ (analytical pure, Aladdin), $YbCl_3 \cdot 6H_2O$ (analytical pure, Aladdin), $ErCl_3 \cdot 6H_2O$ (analytical pure, Aladdin), $HoCl_3 \cdot 6H_2O$ (analytical pure, Aladdin), hydrochloric acid (HCl, analytical pure, Chengdu Kelong Chemical Reagent Factory, China).

2. Synthesis of CAIC DPSCs

To grow pristine CAIC crystals, solid CsCl (0.337 mg, 2.00 mmol), $InCl_3$ (0.221 mg, 1.00 mmol) and AgCl (0.143 mg, 1.00 mmol) were dissolved in 15 ml of 10 M HCl and then transfer into a 50 cm^3 Teflon autoclave. The solution was heated at 150 ℃ for 12 h and then slowly and steadily cooled to 60 °C with a speed of 3 °C per hour and kept a constant temperature of 60 °C in a Teflon-lined stainless steel autoclave. The as-prepared crystals were filtered out and washed with isopropanol and dried in a furnace 3 h at 60 °C.

3. Synthesis of CAIC: x%Cr^{3+} (x=10, 20, 30, 40, and 50)

The synthesis method used is similar to the CAIC DPSCs except for adding different amount of $CrCl_3 \cdot 6H_2O$ with molar ratio of Cr/(Cr + In) as 0.1, 0.2, 0.3, 0.4, 0.5. The corresponding samples are noted as CAIC: x% Cr^{3+} (x=10, 20, 30, 40, and 50)

4. Synthesis of CAIC: 30%Cr^{3+}, y% Yb^{3+} (y=0, 1, 2, 3)

The synthesis method is similar to that for CAIC:Cr^{3+} DPSCs except with different amount of $YbCl_3 \cdot 6H_2O$ with the molar ration of Yb/(Yb+ Cr + In) as 0.01, 0.02, 0.03

and the amount of $CrCl_3 \cdot 6H_2O$ was fixed as the molar ratio of Cr/(Cr + In) of 0.3. The corresponding samples are noted as CAIC:30% Cr^{3+}, y%Yb^{3+} (y= 0, 1, 2, 3)

5. LED fabrication and evaluation

NIR pc-LEDs were fabricated by combining as-synthesized NIR-emitting phosphor CAIC:Cr^{3+},Yb^{3+} with InGaN UV chips (λ_{em}=365 nm). The phosphor was mixed with epoxy resin thoroughly in a weight ratio of 1:1, then was coated on the surface of the chip to make NIR pc-LED. The Electroluminescence (EL) and NIR output power were measured by Spectrum TEQ-EL series electroluminescence quantum efficiency measurement system of Ocean Optics.

6. Characterization

The powders used were all obtained by grinding in a mortar. DX-2700A measured the X-ray diffraction patterns with the Cu Kα radiation. X-ray photoelectron spectroscopy (XPS) was measured by Escalab250Xi X-ray photoelectron spectrometer of Thermo Fisher Scientific Company in the United States. The morphology and size of the DPSCs were characterized by Scanning Electron Microscope (SEM). The elemental composition and distribution of the materials was observed by energy-dispersive X-ray spectroscopy (EDS) coupled to SEM. UV-vis diffuse reflectance spectra of the perovskite powder were obtained at room temperature using the Techcomp UV2600 variable slit UV-vis spectrophotometer. PL, PLE, TRPL, and Temperature-dependent PL were measured by FLS1000 fluorescence spectrometer of Edinburgh instruments. PL and PLE were measured with the xenon lamp (Xe900) as excitation source, TRPL spectrum was recorded with microsecond lamp as an excitation source. PLQY was measured by integrating sphere and Hamamatsu quantum yield measurement system.

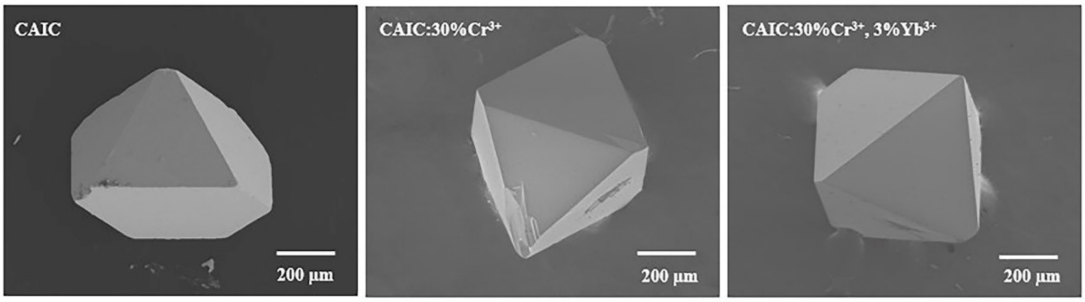

Figure S1. SEM image of CAIC:30%Cr^{3+} and CAIC:30%Cr^{3+}, 3%Yb^{3+}

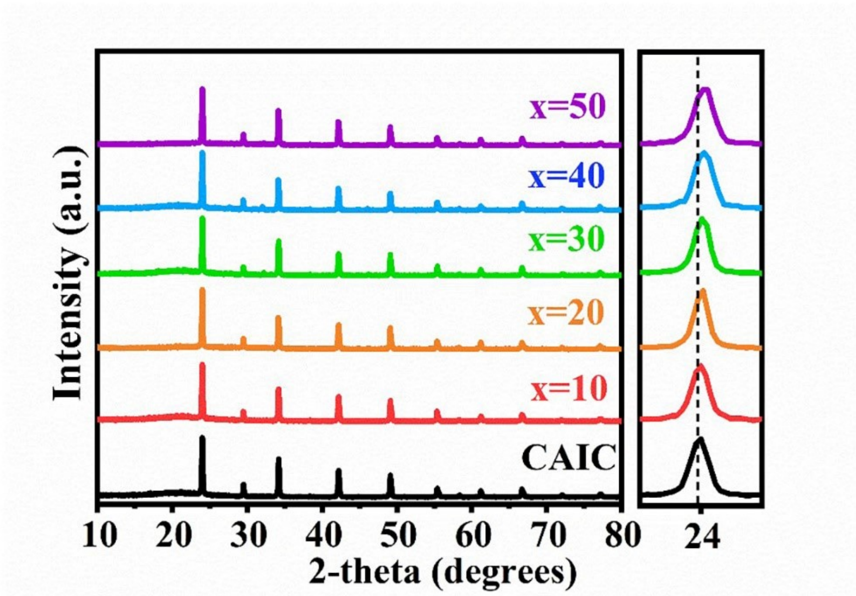

Figure S2. XRD patterns of CAIC: x%Cr^{3+}(x = 0, 10, 20, 30, 40, 50) DPSCs.

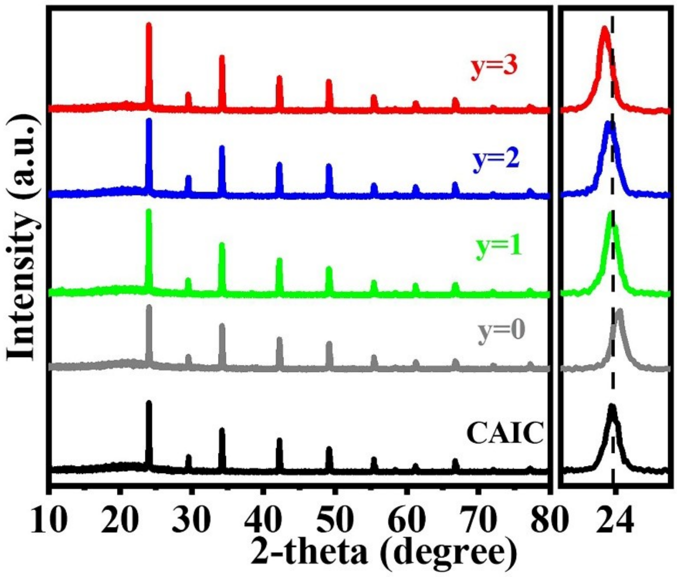

Figure S3. XRD patterns of CAIC:30%Cr, y%Yb (y = 0, 1, 2, 3) DPSCs.

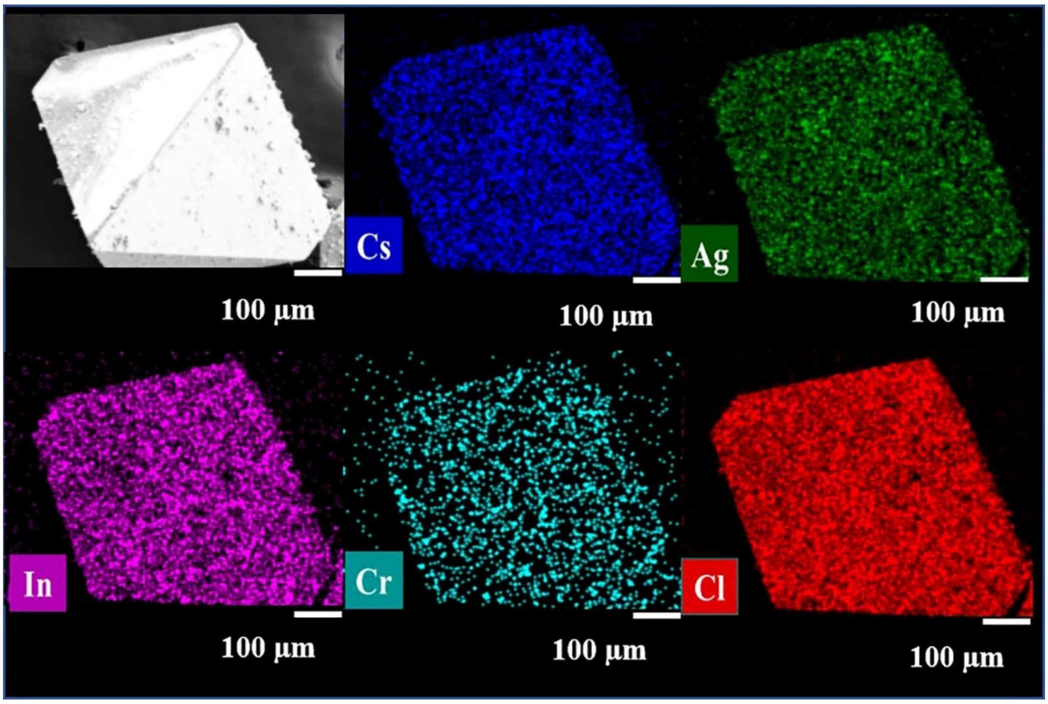

Figure S4. SEM image and EDS spectra of CAIC:30%Cr with the corresponding atomic maps.

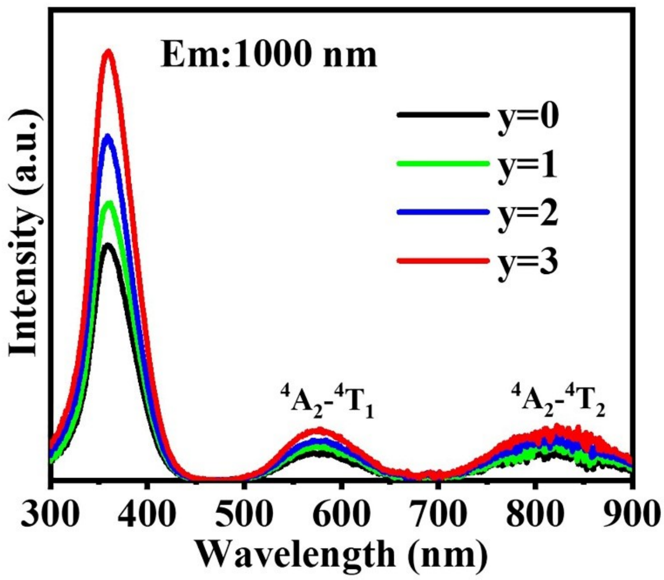

Figure S5. PLE spectra of CAIC:30%Cr^{3+},y%Yb^{3+} (y=0, 1, 2, 3).

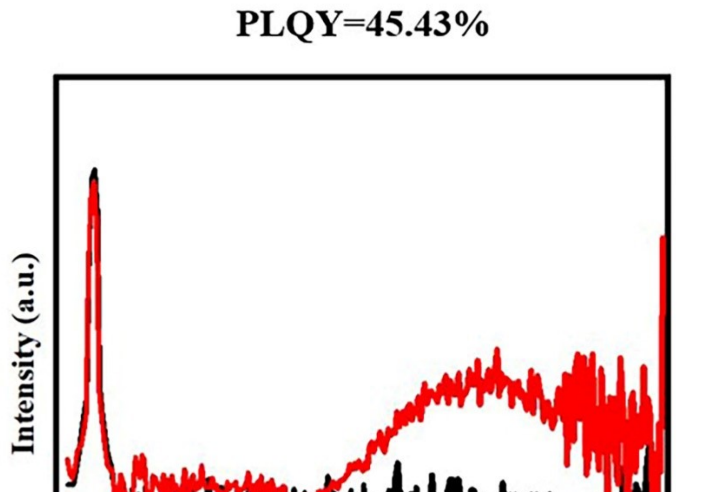

Figure S6. Absolute photoluminescence quantum yield (PLQY) of CAIC:30%Cr^{3+}, 3%Yb^{3+} DPSCs.

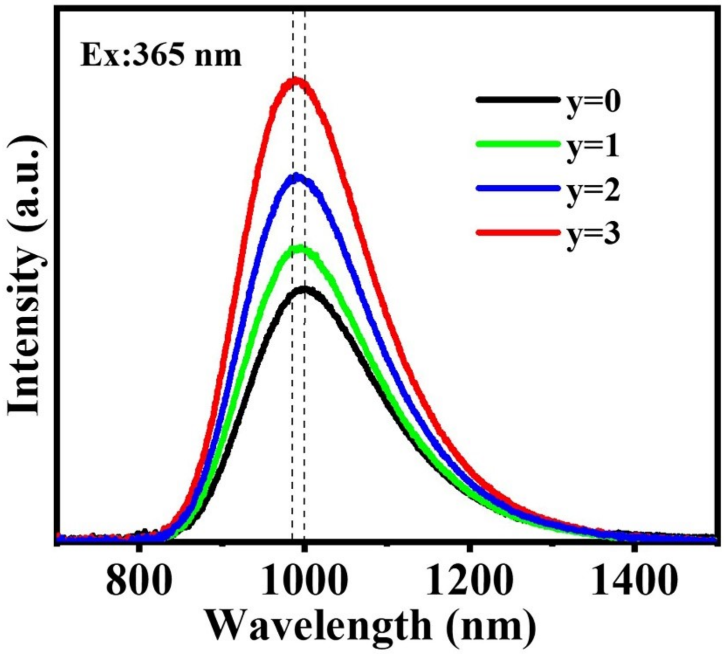

Figure S7. PL spectra of CAIC:30%Cr^{3+},y%Yb^{3+} (y=0, 1, 2, 3). The incorporated samples were tested at λ_{ex}= 365 nm.

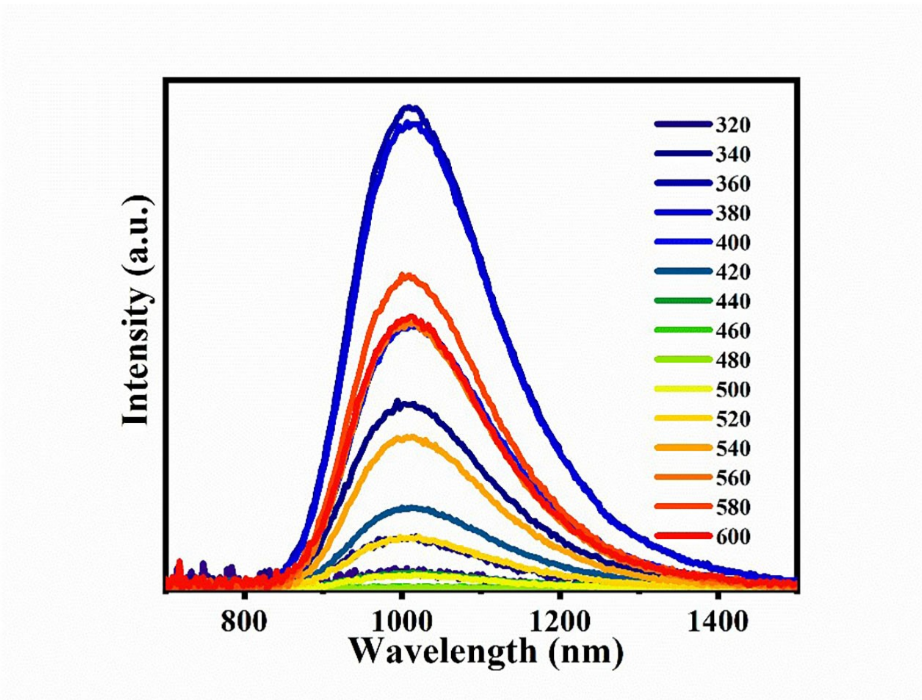

Figure S8. Excitation-wavelength-dependent (320-600 nm) PL spectra of CAIC:30%Cr^{3+},3%Yb^{3+}.

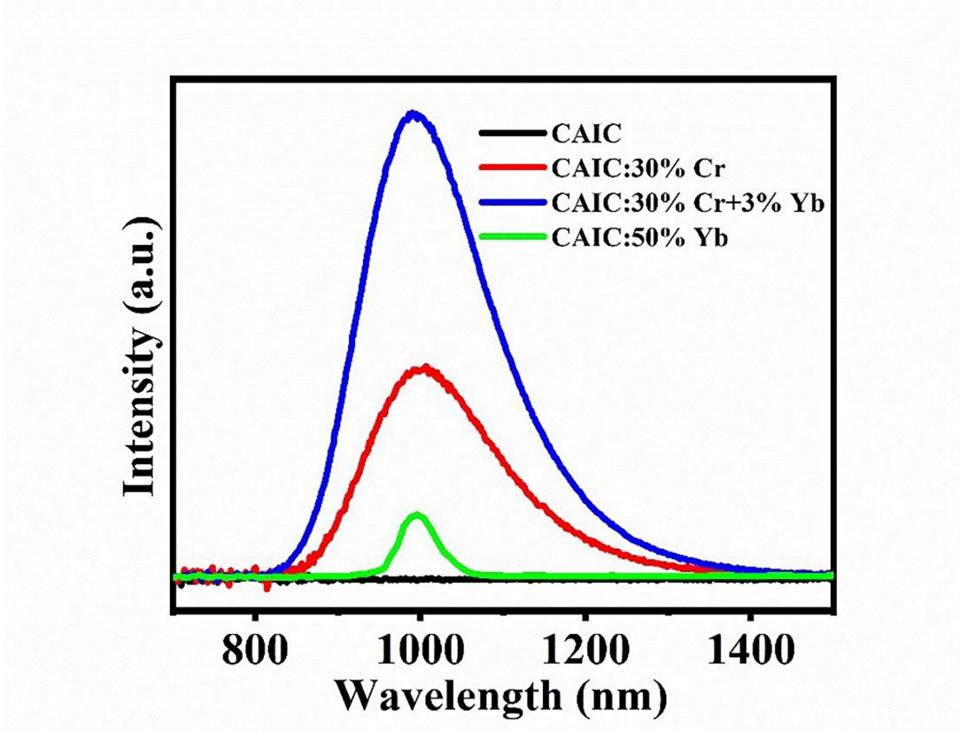

Figure S9. PL spectra of CAIC:30%Cr^{3+},3%Yb^{3+} and CAIC:Yb^{3+}. The emission spectrum of CAIC:Yb^{3+} in the figure is magnified tenfold.

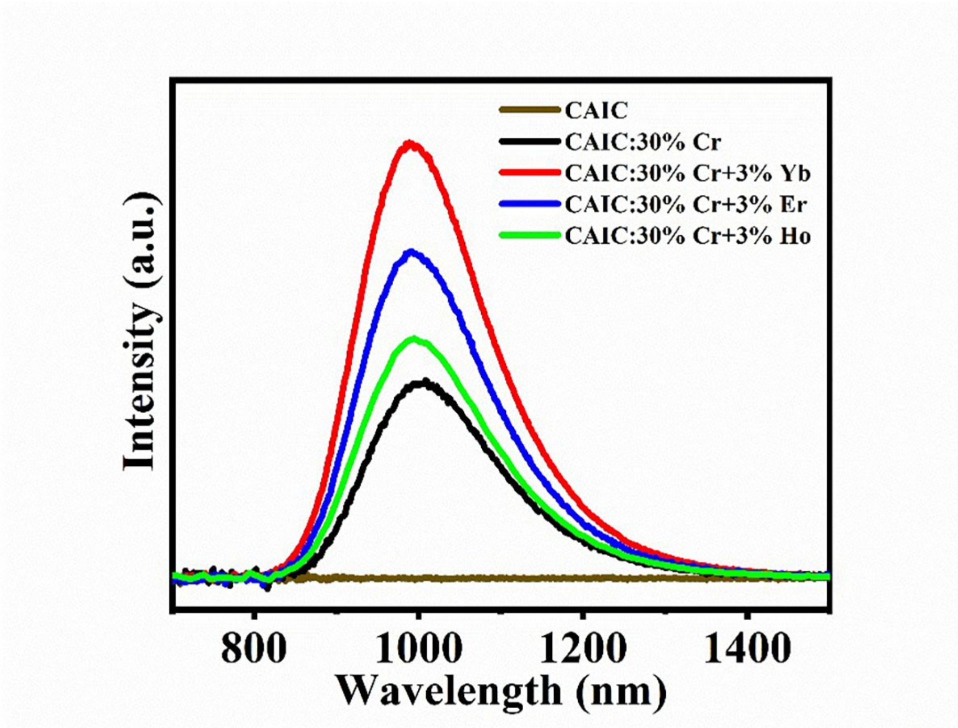

Figure S10. PL curves measured from CAIC:Cr^{3+} and CAIC:Ln^{3+} samples. The incorporated samples were tested at λ_{ex}= 365 nm.

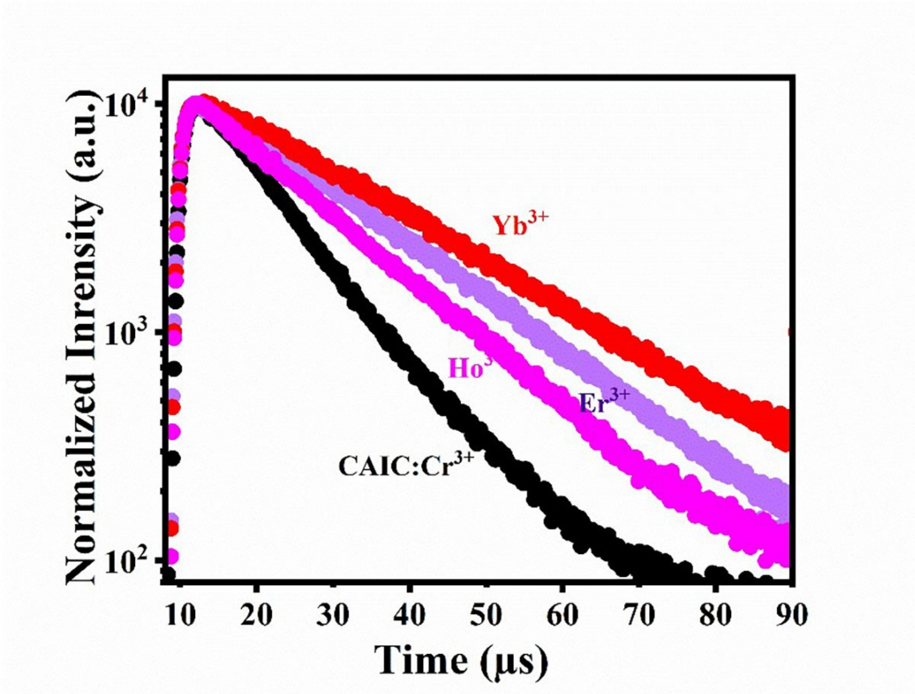

Figure S11. TRPL decay curves of CAIC:Cr^{3+} doped with or without Ln^{3+} ions.

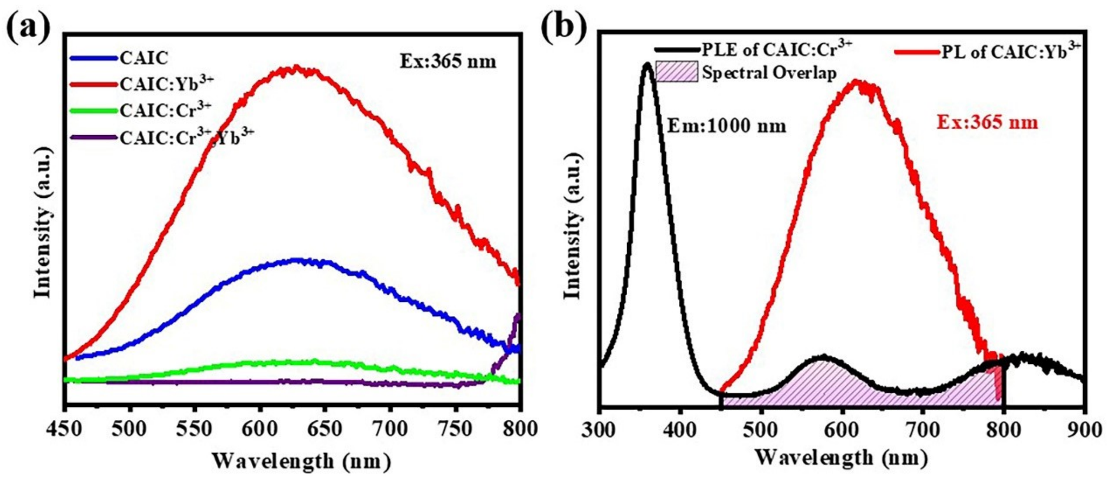

Figure S12. (a) The PL spectra of CAIC:Yb^{3+}, CAIC:Cr^{3+} and CAIC:Cr^{3+},Yb^{3+} at 450-800nm. (b) The spectral overlapping between the PL spectrum of CAIC:Yb^{3+} and the excitation band of CAIC:Cr^{3+}.

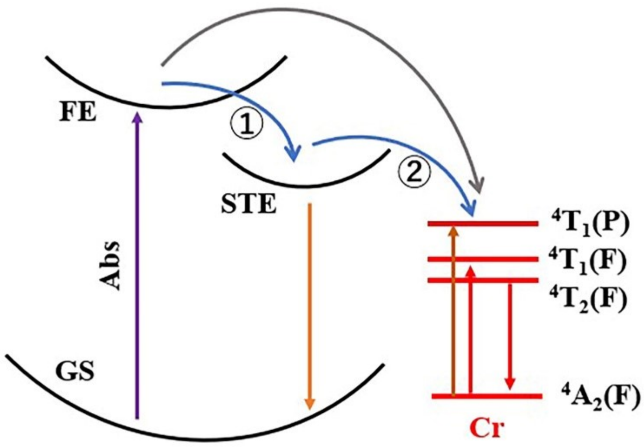

Figure S13. The photophysical process in Cr^{3+}-incorporated CAIC DPSCs.

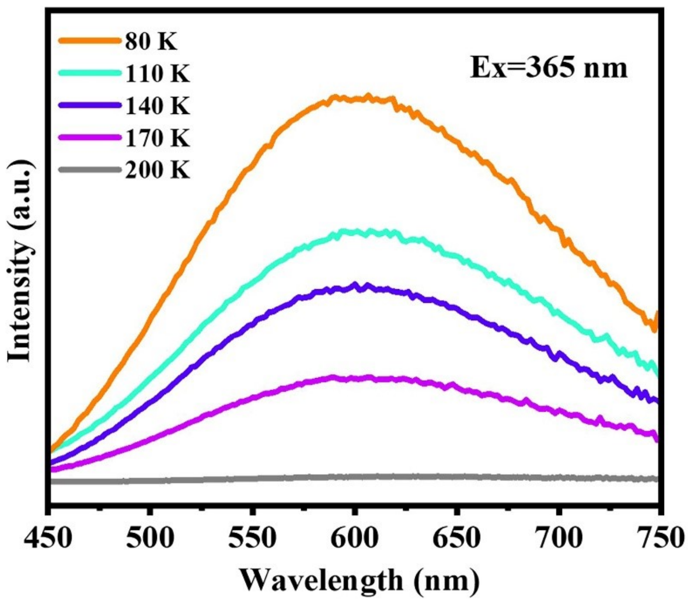

Figure S14. Temperature-dependent PL spectra at 450-750 nm at low temperature of CAIC:Cr^{3+}

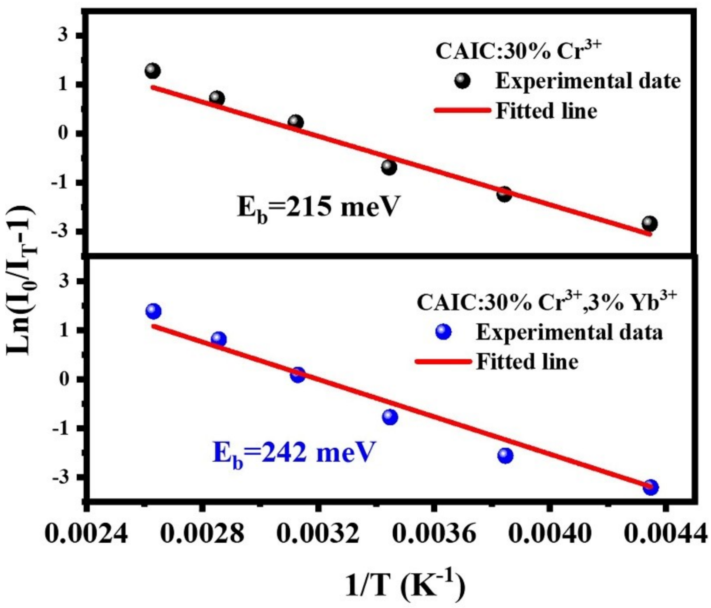

Figure S15. $Ln(I_0/I_T{-}1)$ versus 1/T plot of the temperature dependent spectra.

Table S1 Details of X-ray crystallographic parameters of single crystals.

Parameter	$Cs_2AgIn_{0.7}Cr_{0.3}Cl_6$	$Cs_2AgInCl_6$
Formula weight	628.36	701.21
Crystal system	cubic	cubic
Space group	Fm-3m	Fm-3m
Unit-cell dimension	a/Å=10.4523 b/Å=10.4523 c/Å=10.4523 α/°=90 β/°=90 γ/°=90	a/Å=10.4609 b/Å=10.4609 c/Å=10.4609 α/°=90 β/°=90 γ/°=90
Volume/Å3	1141.9	1144.7
Z	4	2
ρ_{calc} g/cm^3	3.969	4.069
Crystal size/mm^3	0.12 × 0.1 × 0.1	0.2 × 0.2 × 0.2
Radiation	GaKα (λ = 1.34139)	GaKα (λ = 1.34139)
Final R indexes [I>=2σ (I)]	R_1 = 0.0426, wR_2 = 0.0970	R_1 = 0.0255, wR_2 = 1.178
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.0976	R_1 = 0.0255, wR_2 = 0.0513
Largest diff. peak/hole / e Å^{-3}	1.96/-1.27	2.18/−0.74

Table S2. Details of atoms occupation situation of $Cs_2AgIn_{0.7}Cr_{0.3}Cl_6$ single crystal.

Atom	x	y	z	U
Cs1	0.75	0.25	0.25	0.0396
Ag1	0.5	0.5	0.5	0.0273
In1	1	0.5	0.5	0.0276
Cr1	1	0.5	0.5	0.0276
Cl1	0.7402(5)	0.5	0.5	0.0424

Table S3. Bond length of $Cs_2AgIn_{0.7}Cr_{0.3}Cl_6$ single crystal.

Atom	Atom	Length/ **Å**	Atom	Atom	Length/ **Å**
Cs1	Cl1	3.6969(7)	Ag1	$Cl1^{2}$	2.510(5)
Cs1	$Cl1^{1}$	3.6969(7)	Ag1	$Cl1^{12}$	2.510(5)
Cs1	$Cl1^{2}$	3.6969(7)	Ag1	$Cl1^{13}$	2.510(5)
Cs1	$Cl1^{3}$	3.6969(7)	Ag1	$Cl1^{3}$	2.510(5)
Cs1	$Cl1^{4}$	3.6969(7)	Ag1	$Cl1^{14}$	2.510(5)
Cs1	$Cl1^{5}$	3.6969(6)	In1	Cl1	2.716(5)
Cs1	$Cl1^{6}$	3.6969(7)	In1	$Cl1^{15}$	2.716(5)
Cs1	$Cl1^{7}$	3.6969(7)	In1	$Cl1^{1}$	2.716(5)
Cs1	$Cl1^{8}$	3.6969(7)	In1/ Cr1	$Cl1^{16}$	2.716(5)
Cs1	$Cl1^{9}$	3.6969(7)	In1/ Cr1	$Cl1^{8}$	2.716(5)
Cs1	$Cl1^{10}$	3.6969(7)	In1/ Cr1	$Cl1^{17}$	2.716(5)
Cs1	$Cl1^{11}$	3.6969(7)	In1/ Cr1	Cl1	2.716(5)
Ag1	Cl1	2.510(5)			

Table S4. Bond Angles of $Cs_2AgIn_{0.7}Cr_{0.3}Cl_6$ single crystal.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	Cs1	$Cl1^{1}$	119.975(3)	$Cl1^{16}$	Ag1	$Cs1^{12}$	54.736(1)
$Cl1^{2}$	Cs1	$Cl1^{3}$	90.044(5)	$Cl1^{16}$	Ag1	$Cs1^{14}$	125.3
$Cl1^{4}$	Cs1	$Cl1^{5}$	119.974(3)	$Cl1^{7}$	Ag1	$Cl1^{17}$	180.0
$Cl1^{5}$	Cs1	$Cl1^{3}$	176.81(17)	$Cl1^{18}$	Ag1	Cl1	180.0
$Cl1^{6}$	Cs1	$Cl1^{7}$	90.044(5)	$Cl1^{16}$	Ag1	$Cl1^{17}$	90.000(1)
$Cl1^{8}$	Cs1	$Cl1^{5}$	62.60(13)	$Cl1^{17}$	Ag1	Cl1	90.000(1)
$Cl1^{8}$	Cs1	$Cl1^{3}$	119.974(3)	$Cl1^{10}$	Ag1	$Cl1^{7}$	90.0
Cl1	Cs1	$Cl1^{2}$	176.81(17)	$Cl1^{16}$	Ag1	$Cl1^{7}$	90.0
$Cl1^{1}$	Cs1	$Cl1^{7}$	90.044(5)	$Cl1^{7}$	Ag1	$Cl1^{18}$	90.000(1)
$Cl1^{4}$	Cs1	$Cl1^{7}$	119.974(3)	$Cl1^{10}$	Ag1	$Cl1^{18}$	90.000(1)
Cl1	Cs1	$Cl1^{5}$	90.044(5)	$Cl1^{17}$	Ag1	$Cl1^{18}$	90.0
$Cl1^{1}$	Cs1	$Cl1^{2}$	57.39(14)	$Cl1^{10}$	Ag1	$Cl1^{16}$	180.0
$Cl1^{9}$	Cs1	$Cl1^{5}$	119.974(3)	$Cl1^{10}$	Ag1	Cl1	90.0
$Cl1^{1}$	Cs1	$Cl1^{3}$	62.60(13)	$Cl1^{16}$	Ag1	$Cl1^{18}$	90.0
$Cl1^{2}$	Cs1	$Cl1^{9}$	62.60(13)	$Cl1^{16}$	Ag1	Cl1	90.000(1)
Cl1	Cs1	$Cl1^{8}$	119.975(3)	$Cl1^{7}$	Ag1	Cl1	90.0
$Cl1^{10}$	Cs1	$Cl1^{9}$	119.974(3)	$Cl1^{10}$	Ag1	$Cl1^{17}$	90.0
Cl1	Cs1	$Cl1^{7}$	57.39(14)	$Cs1^{19}$	In1	$Cs1^{20}$	70.5
$Cl1^{8}$	Cs1	$Cl1^{7}$	62.60(13)	$Cs1^{21}$	In1	$Cs1^{5}$	109.471(1)
$Cl1^{1}$	Cs1	$Cl1^{8}$	57.39(14)	$Cs1^{21}$	In1	$Cs1^{19}$	109.471(1)

Cl1^{10}	Cs1	Cl1^{7}	57.39(14)	Cs1	In1	Cs1^{5}	70.529(1)
Cl1^{9}	Cs1	Cl1^{7}	176.81(17)	Cs1^{21}	In1	Cs1^{3}	109.471(1)
Cl1^{2}	Cs1	Cl1^{5}	90.044(5)	Cs1^{5}	In1	Cs1^{3}	109.471(1)
Cl1^{2}	Cs1	Cl1^{8}	57.39(14)	Cs1^{5}	In1	Cs1^{20}	180.0
Cl1^{11}	Cs1	Cl1^{5}	57.39(14)	Cs1	In1	Cs1^{21}	180.0
Cl1^{10}	Cs1	Cl1^{5}	119.974(3)	Cs1^{3}	In1	Cs1^{20}	70.5
Cl1	Cs1	Cl1^{3}	90.044(5)	Cs1	In1	Cs1^{3}	70.529(1)
Cl1	Cs1	Cl1^{4}	62.60(13)	Cs1	In1	Cs1^{19}	70.529(1)
Cl1^{1}	Cs1	Cl1^{9}	90.044(5)	Cs1^{21}	In1	Cs1^{20}	70.529(1)
Cl1^{11}	Cs1	Cl1^{3}	119.974(3)	Cs1	In1	Cs1^{20}	109.5
Cl1^{8}	Cs1	Cl1^{9}	119.974(3)	Cs1^{19}	In1	Cs1^{3}	109.5
Cl1^{1}	Cs1	Cl1^{4}	119.974(3)	Cs1^{19}	In1	Cs1^{5}	109.5
Cl1^{1}	Cs1	Cl1^{11}	119.974(3)	Cl1^{22}	In1	Cs1^{19}	125.3
Cl1^{11}	Cs1	Cl1^{9}	62.60(13)	Cl1^{22}	In1	Cs1^{3}	54.736(1)
Cl1^{2}	Cs1	Cl1^{11}	62.60(13)	Cl1^{23}	In1	Cs1^{20}	125.264(1)
Cl1^{2}	Cs1	Cl1^{4}	119.974(3)	Cl1^{6}	In1	Cs1^{19}	54.7
Cl1^{8}	Cs1	Cl1^{11}	90.044(5)	Cl1	In1	Cs1	54.7
Cl1^{2}	Cs1	Cl1^{7}	119.974(2)	Cl1^{21}	In1	Cs1^{5}	125.3
Cl1^{4}	Cs1	Cl1^{11}	90.044(5)	Cl1	In1	Cs1^{3}	54.7
Cl1^{8}	Cs1	Cl1^{4}	176.81(17)	Cl1^{6}	In1	Cs1	54.7
Cl1^{6}	Cs1	Cl1^{11}	57.39(14)	Cl1^{21}	In1	Cs1^{3}	125.3
Cl1^{11}	Cs1	Cl1^{7}	119.974(3)	Cl1^{21}	In1	Cs1^{21}	54.7
Cl1	Cs1	Cl1^{10}	57.39(14)	Cl1^{23}	In1	Cs1^{19}	125.3
Cl1	Cs1	Cl1^{6}	62.60(13)	Cl1^{21}	In1	Cs1	125.3
Cl1^{1}	Cs1	Cl1^{10}	62.60(13)	Cl1^{21}	In1	Cs1^{20}	54.7
Cl1^{1}	Cs1	Cl1^{5}	119.974(2)	Cl1^{6}	In1	Cs1^{20}	125.3
Cl1^{2}	Cs1	Cl1^{10}	119.974(3)	Cl1^{4}	In1	Cs1^{5}	125.3
Cl1^{1}	Cs1	Cl1^{6}	176.81(17)	Cl1	In1	Cs1^{21}	125.3
Cl1^{8}	Cs1	Cl1^{10}	90.044(5)	Cl1^{22}	In1	Cs1^{5}	125.3
Cl1^{6}	Cs1	Cl1^{5}	57.39(14)	Cl1^{6}	In1	Cs1^{3}	125.3
Cl1^{4}	Cs1	Cl1^{10}	90.044(5)	Cl1^{6}	In1	Cs1^{5}	54.7
Cl1^{2}	Cs1	Cl1^{6}	119.974(3)	Cl1^{23}	In1	Cs1^{21}	54.736(1)
Cl1^{6}	Cs1	Cl1^{10}	119.974(3)	Cl1^{4}	In1	Cs1^{21}	125.3
Cl1^{7}	Cs1	Cl1^{5}	62.60(13)	Cl1	In1	Cs1^{19}	125.3
Cl1^{11}	Cs1	Cl1^{10}	176.81(17)	Cl1^{22}	In1	Cs1^{21}	54.7
Cl1^{8}	Cs1	Cl1^{6}	119.974(3)	Cl1	In1	Cs1^{5}	54.7
Cl1^{6}	Cs1	Cl1^{3}	119.974(3)	Cl1^{6}	In1	Cs1^{21}	125.3
Cl1^{4}	Cs1	Cl1^{3}	57.39(14)	Cl1^{4}	In1	Cs1^{20}	54.7
Cl1^{10}	Cs1	Cl1^{3}	62.60(13)	Cl1^{4}	In1	Cs1^{19}	54.7
Cl1^{4}	Cs1	Cl1^{6}	62.60(13)	Cl1^{23}	In1	Cs1^{5}	54.736(1)
Cl1^{7}	Cs1	Cl1^{3}	119.974(3)	Cl1^{23}	In1	Cs1	125.264(1)
Cl1^{9}	Cs1	Cl1^{3}	57.39(14)	Cl1^{23}	In1	Cs1^{3}	125.3
Cl1^{4}	Cs1	Cl1^{9}	57.39(14)	Cl1^{4}	In1	Cs1	54.7
Cl1	Cs1	Cl1^{11}	119.974(3)	Cl1^{22}	In1	Cs1	125.3
Cl1^{6}	Cs1	Cl1^{9}	90.044(5)	Cl1^{21}	In1	Cs1^{19}	54.7
Cl1	Cs1	Cl1^{9}	119.974(3)	Cl1^{4}	In1	Cs1^{3}	54.7
Cs1^{12}	Ag1	Cs1^{13}	180.0	Cl1	In1	Cs1^{20}	125.3
Cs1	Ag1	Cs1^{14}	109.5	Cl1^{22}	In1	Cs1^{20}	54.7

Cs1	Ag1	Cs1^{15}	109.5	Cl1	In1	Cl1^{22}	90.000(1)
Cs1^{13}	Ag1	Cs1^{14}	70.529(1)	Cl1^{4}	In1	Cl1^{21}	90.0
Cs1^{12}	Ag1	Cs1^{15}	109.471(1)	Cl1^{22}	In1	Cl1^{6}	180.0
Cs1^{13}	Ag1	Cs1^{15}	70.529(1)	Cl1^{23}	In1	Cl1^{21}	90.000(1)
Cs1^{5}	Ag1	Cs1^{15}	70.5	Cl1	In1	Cl1^{23}	90.000(1)
Cs1^{12}	Ag1	Cs1	109.471(1)	Cl1	In1	Cl1^{4}	90.000(1)
Cs1^{12}	Ag1	Cs1^{5}	70.529(1)	Cl1	In1	Cl1^{6}	90.000(1)
Cs1^{5}	Ag1	Cs1^{14}	180.0	Cl1^{23}	In1	Cl1^{22}	90.000(1)
Cs1^{13}	Ag1	Cs1^{5}	109.5	Cl1^{23}	In1	Cl1^{6}	90.0
Cs1^{13}	Ag1	Cs1	70.529(1)	Cl1^{22}	In1	Cl1^{21}	90.000(1)
Cs1	Ag1	Cs1^{5}	70.5	Cl1^{23}	In1	Cl1^{4}	180.0
Cs1^{12}	Ag1	Cs1^{14}	109.471(1)	Cl1^{4}	In1	Cl1^{22}	90.0
Cs1^{14}	Ag1	Cs1^{15}	109.471(1)	Cl1^{6}	In1	Cl1^{21}	90.0
Cl1^{16}	Ag1	Cs1^{5}	54.7	Cl1	In1	Cl1^{21}	180.0
Cl1^{10}	Ag1	Cs1^{14}	54.7	Cl1^{4}	In1	Cl1^{6}	90.0
Cl1^{7}	Ag1	Cs1^{15}	54.7	Cs1^{12}	Cl1	Cs1	176.81(17)
Cl1^{7}	Ag1	Cs1^{5}	54.7	Cs1	Cl1	Cs1^{5}	89.956(5)
Cl1^{17}	Ag1	Cs1^{13}	125.3	Cs1^{5}	Cl1	Cs1^{3}	176.81(17)
Cl1^{17}	Ag1	Cs1^{12}	54.7	Cs1	Cl1	Cs1^{3}	89.956(5)
Cl1	Ag1	Cs1^{13}	125.3	Cs1^{12}	Cl1	Cs1^{3}	89.956(5)
Cl1^{18}	Ag1	Cs1^{5}	125.3	Cs1^{12}	Cl1	Cs1^{5}	89.956(5)
Cl1^{17}	Ag1	Cs1^{5}	125.3	Ag1	Cl1	Cs1	91.59(8)
Cl1	Ag1	Cs1^{5}	54.7	Ag1	Cl1	Cs1^{5}	91.59(8)
Cl1^{7}	Ag1	Cs1^{12}	125.3	Ag1	Cl1	Cs1^{3}	91.59(8)
Cl1^{18}	Ag1	Cs1^{12}	125.3	Ag1	Cl1	Cs1^{12}	91.59(8)
Cl1^{10}	Ag1	Cs1^{5}	125.3	Ag1	Cl1	In1	180.0
Cl1	Ag1	Cs1^{12}	54.7	Ag1	Cl1	Cr1	180.0
Cl1^{10}	Ag1	Cs1^{13}	54.7	In1	Cl1	Cs1^{3}	88.41(8)
Cl1^{7}	Ag1	Cs1^{14}	125.3	In1	Cl1	Cs1	88.41(8)
Cl1^{7}	Ag1	Cs1	54.7	In1	Cl1	Cs1^{5}	88.41(8)
Cl1	Ag1	Cs1^{14}	125.3	In1	Cl1	Cs1^{12}	88.41(8)
Cl1^{10}	Ag1	Cs1	54.7	Cr1	Cl1	Cs1	88.41(8)
Cl1^{7}	Ag1	Cs1^{13}	54.7	Cl1^{21}	Cr1	Cl1^{22}	90.000(1)
Cl1^{10}	Ag1	Cs1^{15}	125.3	Cl1^{23}	Cr1	Cl1^{4}	180.0
Cl1^{18}	Ag1	Cs1^{13}	54.7	Cl1^{23}	Cr1	Cl1^{21}	90.000(1)
Cl1^{17}	Ag1	Cs1	125.3	Cl1	Cr1	Cl1^{4}	90.000(1)
Cl1^{16}	Ag1	Cs1^{15}	54.736(1)	Cl1	Cr1	Cl1^{21}	180.0
Cl1^{16}	Ag1	Cs1^{13}	125.264(1)	Cl1^{21}	Cr1	Cl1^{4}	90.0
Cl1^{17}	Ag1	Cs1^{15}	125.3	Cl1	Cr1	Cl1^{22}	90.000(1)
Cl1^{18}	Ag1	Cs1	125.3	Cl1^{6}	Cr1	Cl1^{4}	90.0
Cl1	Ag1	Cs1^{15}	125.3	Cl1^{23}	Cr1	Cl1^{22}	90.000(1)
Cl1^{18}	Ag1	Cs1^{15}	54.7	Cl1^{23}	Cr1	Cl1^{6}	90.0
Cl1^{10}	Ag1	Cs1^{12}	125.3	Cl1^{22}	Cr1	Cl1^{4}	90.0
Cl1	Ag1	Cs1	54.7	Cl1^{21}	Cr1	Cl1^{6}	90.0
Cl1^{16}	Ag1	Cs1	125.3	Cl1	Cr1	Cl1^{23}	90.000(1)
Cl1^{18}	Ag1	Cs1^{14}	54.7	Cl1	Cr1	Cl1^{6}	90.000(1)
Cl1^{17}	Ag1	Cs1^{14}	54.7	Cl^{16}	Cr1	Cl1^{22}	180.0

Table S5 Cr^{3+} and Yb^{3+} content from starting materials and measured by ICP.

CAIC:x% Cr^{3+}	
Nominal (atomic ratio %) {[Cr] / ([Cr] + [In])} ×100	ICP-OES (atomic ratio % of Cr) {[Cr] / ([Cr] + [In])} ×100
10	0.0766
20	0.1592
30	0.2814
40	0.4568
50	0.9586

CAIC:30% Cr^{3+},y%Yb	
Nominal (atomic ratio y %) {[Yb] / ([Yb] +[Cr]+ [In])} ×100	ICP-MS (atomic ratio % of Yb) {[Yb] / ([Yb] +[Cr]+ [In])} ×100
3	0.018