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# Supporting information

## Achieving high thermal stability of different rare earth ions in a single matrix host via manipulated the local structure by solid solution

Xiuxia Yang[a], Lei Zhao[b], Zhichao Liu[a], Shuyu Tian[a], Hao Zhang[a], Xuhui Xu[a]*, Jianbei Qiu[a], and Xue Yu[a]*

[a] *College of Materials Science and Engineering, Kunming University of Science and Technology, Kunming 650093, P. R. China*

[b] *School of Physics and Opto-Electronic Technology, Baoji University of Arts and Sciences, Baoji 721016, Shaanxi, P. R. China*

*Corresponding Author: Xue Yu E-mails: yuyu6593@126.com*

*Corresponding Author: Xuhui Xu E-mails: xuxuh07@126.com*

Table S1 The crystallographic data of CAS.

| **Atom** | **Wyck** | **S.O.F.** | **x** | **y** | **z** |
|---|---|---|---|---|---|
| Ca1 | 4e | | 0.3389(1) | 0.1611(1) | 0.51040 |
| Al1 | 2a | | 0 | 0 | 0 |
| Si1 | 4e | 0.5 | 0.1434(1) | 0.3566(1) | 0.9540(2) |
| Al2 | 4e | 0.5 | 0.1434(1) | 0.3566(1) | 0.9540(2) |
| O1 | 2c | | 1/2 | 0 | 0.1765(2) |
| O2 | 4e | | 0.1427(1) | 0.3573(1) | 0.2835(1) |
| O3 | 8f | | 0.0876(1) | 0.1678(1) | 0.8078(1) |

Table S2 The crystallographic data of CYA.

| **Atom** | **Wyck** | **S.O.F.** | **x** | **y** | **z** |
|---|---|---|---|---|---|
| Ca1 | 4e | 0.5 | 0.3379(2) | 0.16210 | 0.5098(9) |
| Y1 | 4e | 0.5 | 0.3379(2) | 0.16210 | 0.5098(9) |
| Al1 | 2a | | 0 | 0 | 0 |
| Al2 | 4e | | 0.1441(5) | 0.35590 | 0.9555(13) |

| | | | | |
|---|---|---|---|---|
| O1 | 2c | 1/2 | 0 | 0.192(3) |
| O2 | 4e | 0.1403(13) | 0.35930 | 0.299(2) |
| O3 | 8f | 0.0878(11) | 0.1658(10) | 0.794(2) |

Table S3 Selected bond distances of CAS and CYA.

| **$Ca_2Al_2SiO_7$** | | **$CaYAl_3O_7$** | |
|---|---|---|---|
| Ca1-O3 | 2.825Å | Ca1/Y1-O3 | 2.849Å |
| Ca1-O3 | 2.825Å | Ca1/Y1-O3 | 2.849Å |
| Ca1-O3 | 2.450Å | Ca1/Y1-O3 | 2.319Å |
| Ca1-O3 | 2.450Å | Ca1/Y1-O3 | 2.319Å |
| Ca1-O2 | 2.422Å | Ca1/Y1-O2 | 2.413Å |
| Ca1-O2 | 2.561Å | Ca1/Y1-O2 | 2.502Å |
| Ca1-O2 | 2.561Å | Ca1/Y1-O2 | 2.502Å |
| Ca1-O1 | 2.434Å | Ca1/Y1-O1 | 2.382Å |

Table S4 Crystallographic parameters gained form rietveld refinement results for CAS and CAS: $Tb^{3+}$.

| Formula | CAS | CAS: 0.01$Tb^{3+}$ |
|---|---|---|
| Symmetry | tetragonal | tetragonal |
| Space group | P-421 m | P-421 m |
| a/Å | 7.800058 | 7.677734 |
| b/Å | 7.800058 | 7.677734 |
| c/Å | 5.147901 | 5.065137 |
| β/degree | 90 | 90 |
| Volume/$Å^3$ | 313.203 | 298.578 |
| Rwp | 13.59 | 14.35 |
| Rp | 10.08 | 12.06 |
| $\chi^2$ | 2.63 | 2.85 |

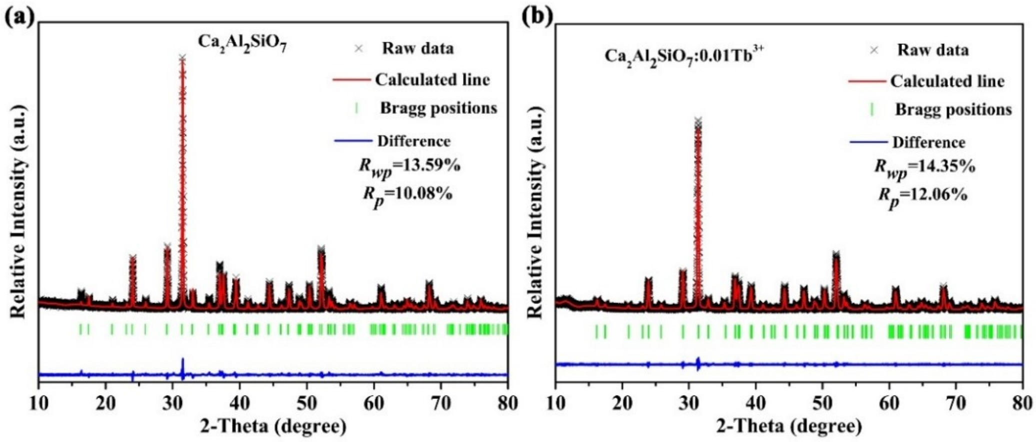


Figure. S1 XRD refinement results of CAS (a) and CAS: 0.01$Tb^{3+}$ (b), respectively.

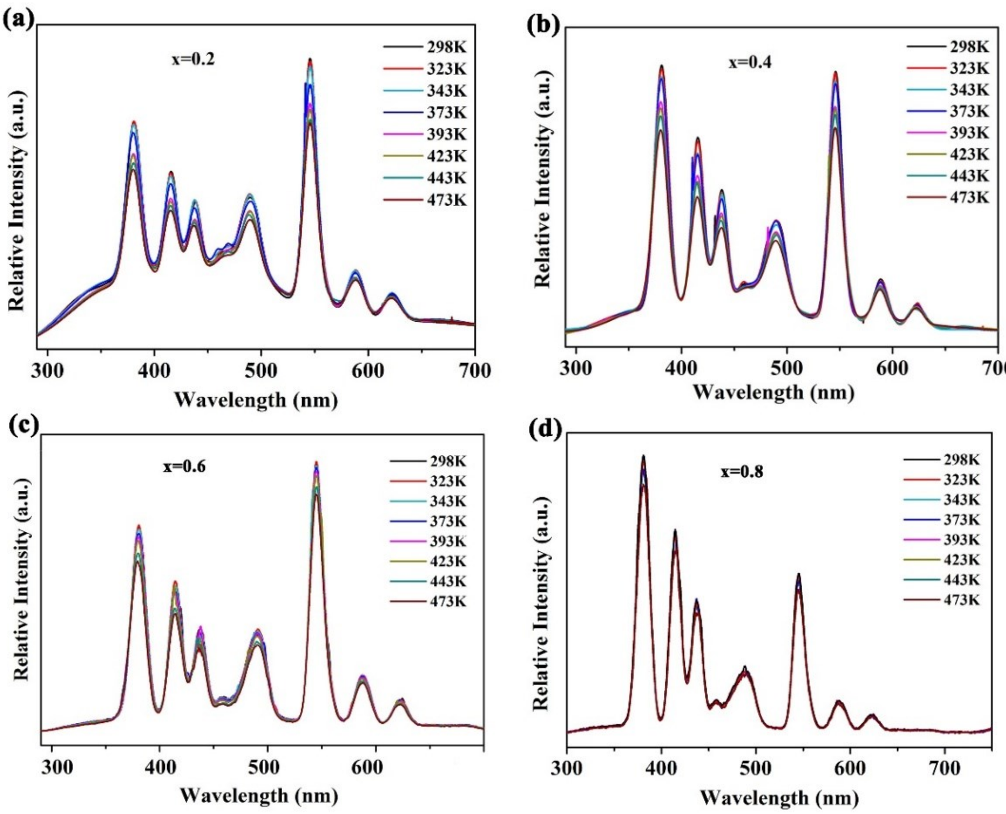


Figure. S2 Temperature-dependent PL spectra of $Ca_{2-x}Y_xAl_2Si_{1-x}Al_xO_7$: 0.01$Tb^{3+}$ (x=0.2 (a), 0.4 (b), 0.6 (c), 0.8 (d)), respectively.

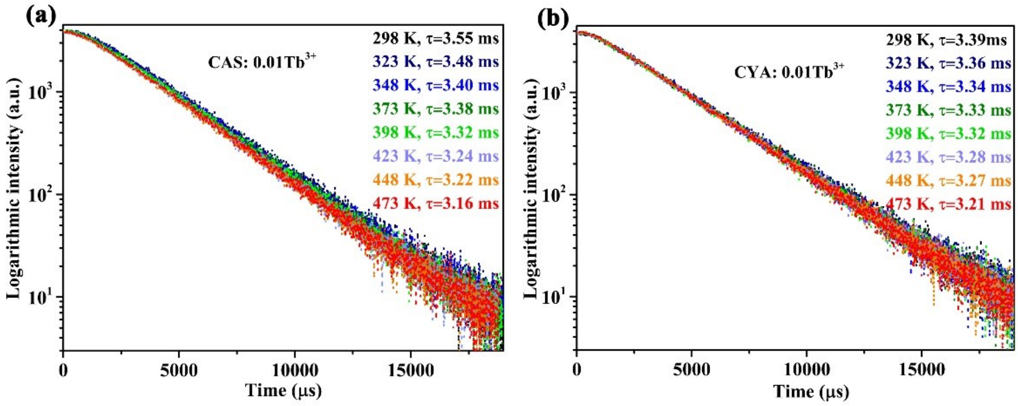


Figure. S3 Temperature-dependent decay curves of PL spectra of CAS: $0.01Tb^{3+}$ (a) and CYA: $0.01Tb^{3+}$ (b).

The fluorescence decay curves are fitted by a double-exponential function:

$$I(t) = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right)$$

where t is the time, I(t) is the corresponding luminescence intensity, $A_1$ and $A_2$ are constants, and $\tau_1$ and $\tau_2$ are the rapid and slow decay times for the exponential components, respectively. Based on the fitted parameters, the value of the average lifetime $\tau$ can be acquired utilizing the following expression:

$$\tau = \frac{A_1{\tau_1}^2 + A_1{\tau_2}^2}{A_1\tau_1 + A_1\tau_2}$$

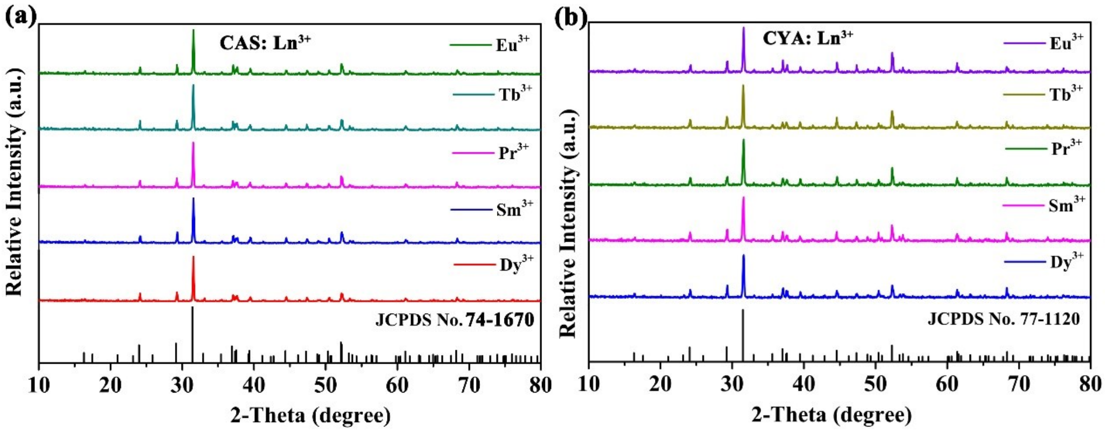


Figure. S4 XRD patterns of CAS: $0.01Ln^{3+}$ (a), CYA: $0.01Ln^{3+}$ ($Eu^{3+}$, $Tb^{3+}$, $Sm^{3+}$, $Dy^{3+}$, and $Pr^{3+}$) (b) and the standard patterns of CAS (JCPDS No. 74-1670) and CYA (JCPDS No. 77-1120), respectively.

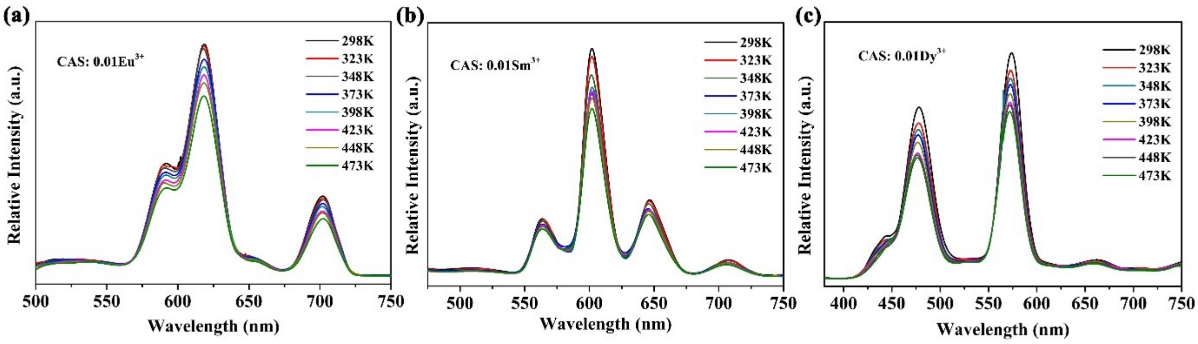


Figure. S5 The temperature-dependent PL spectra of CAS: $0.01Ln^{3+}$ ($Eu^{3+}$ (a), $Sm^{3+}$ (b), $Dy^{3+}$ (c)).

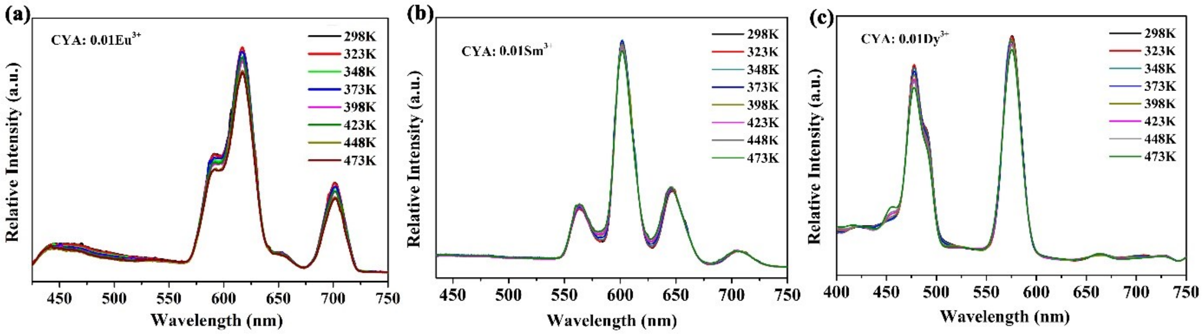


Figure. S6 The temperature-dependent PL spectra of CAS: 0.01Ln$^{3+}$ (Eu$^{3+}$ (a), Sm$^{3+}$ (b), Dy$^{3+}$ (c)).

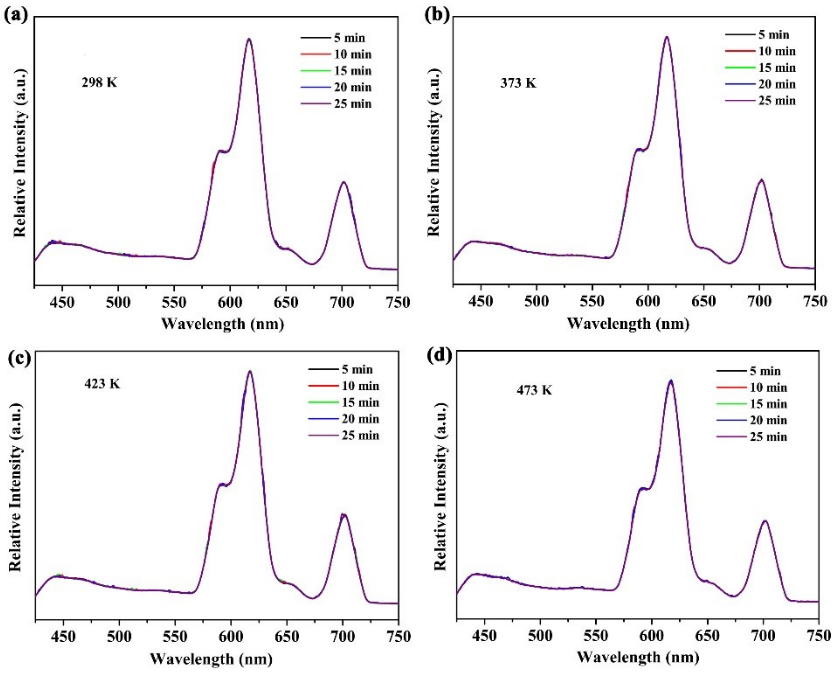


Figure. S7 PL spectra of CYA: 0.01Eu$^{3+}$ at different duration time and ambient temperature.

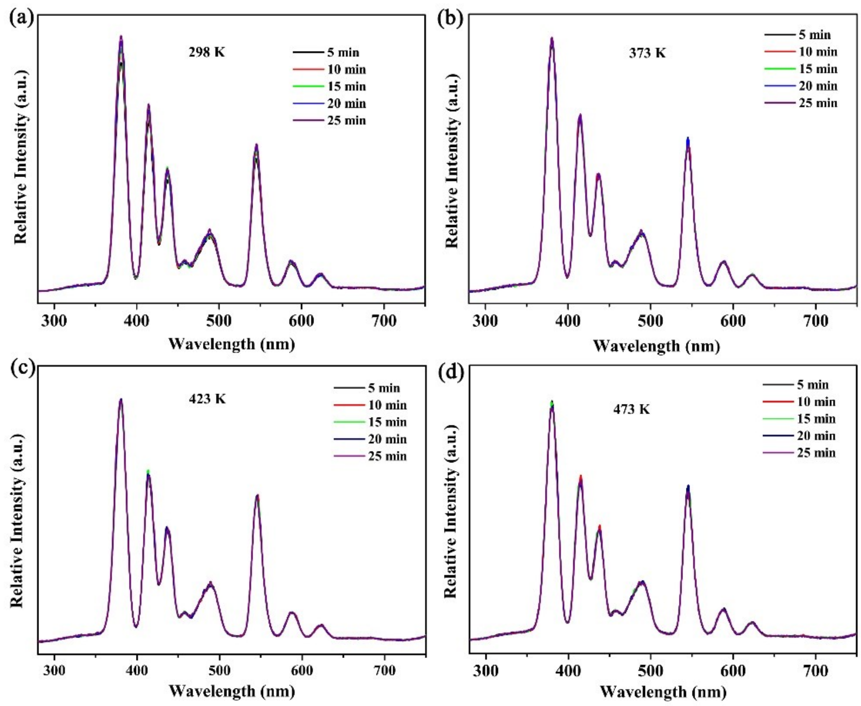


Figure. S8 PL spectra of CYA: $0.01Tb^{3+}$ at different duration time and ambient temperature.

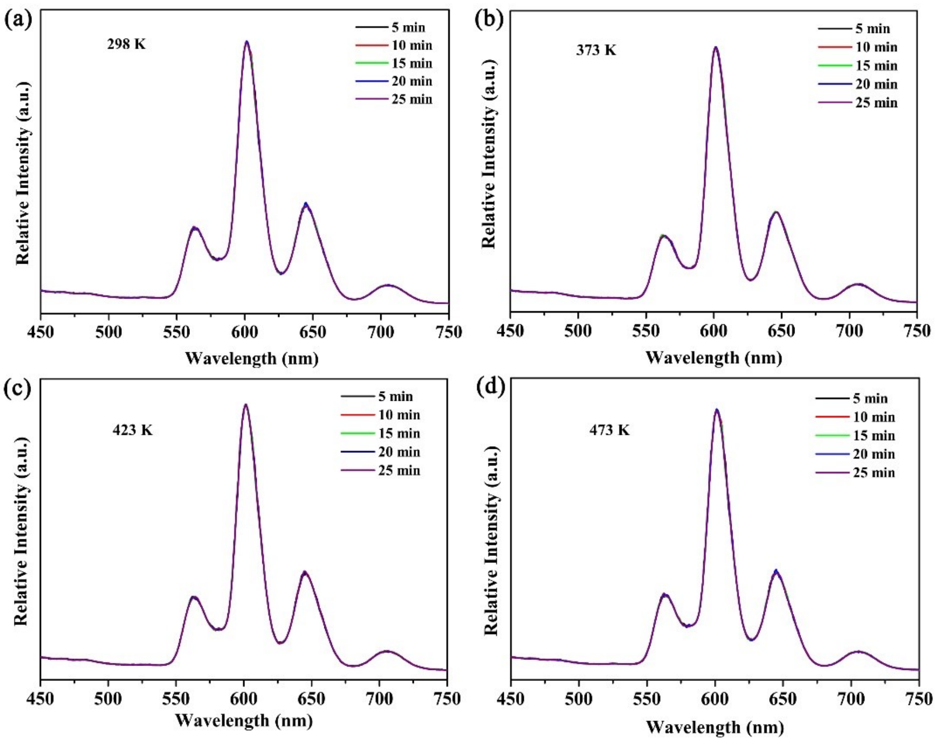


Figure. S9 PL spectra of CYA: $0.01Sm^{3+}$ at different duration time and ambient temperature.

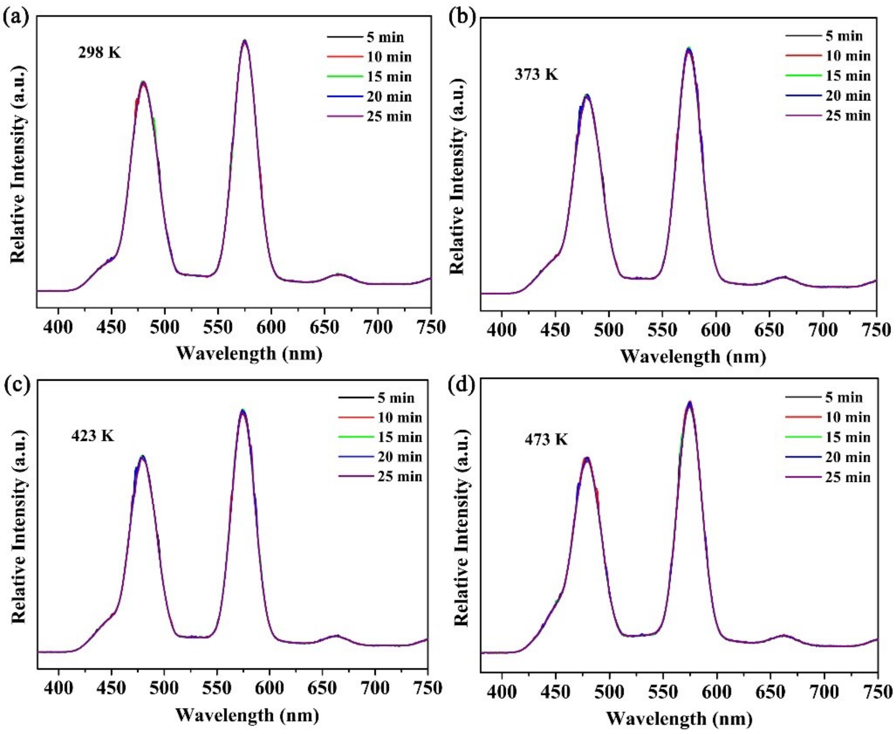


Figure. S10 PL spectra of CYA: $0.01Dy^{3+}$ at different duration time and ambient temperature.

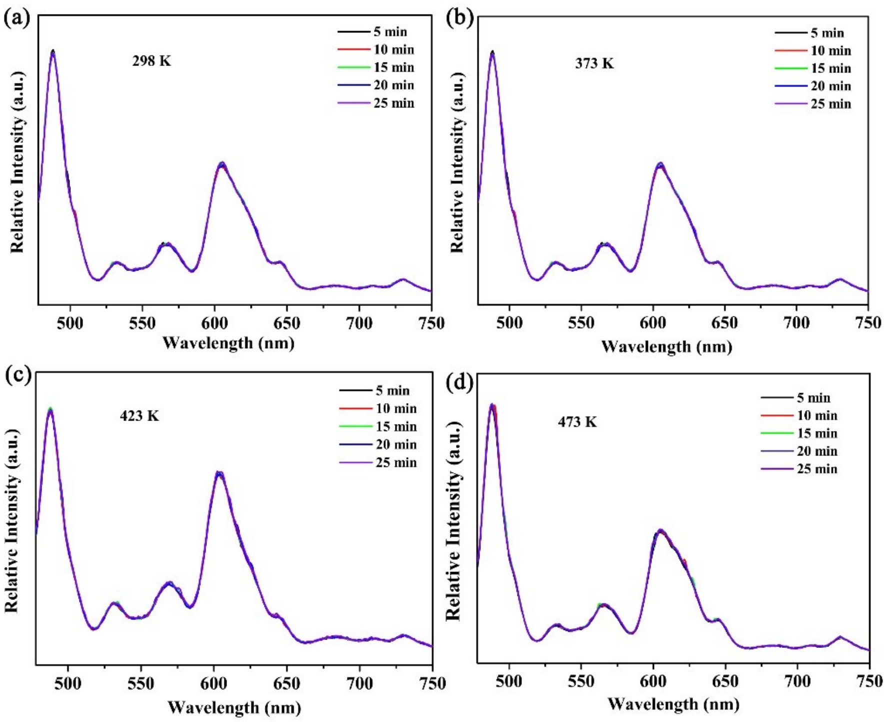


Figure. S11 PL spectra of CYA: $0.01Pr^{3+}$ at different duration time and ambient temperature.

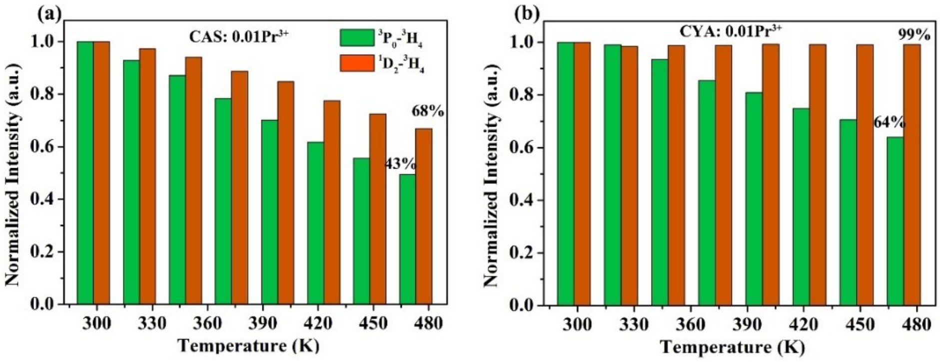


Figure. S12 Temperature-dependent emission intensity of $^3P_0$ and $^1D_2$ emission of CAS: $0.01Pr^{3+}$ (a) and CYA: $0.01Pr^{3+}$ (b) under the excitation of 450 nm.