

Supporting Information

Double Perovskite Cs₂AgInCl₆:Cr³⁺: a Broadband and Near-infrared Luminescent Materials

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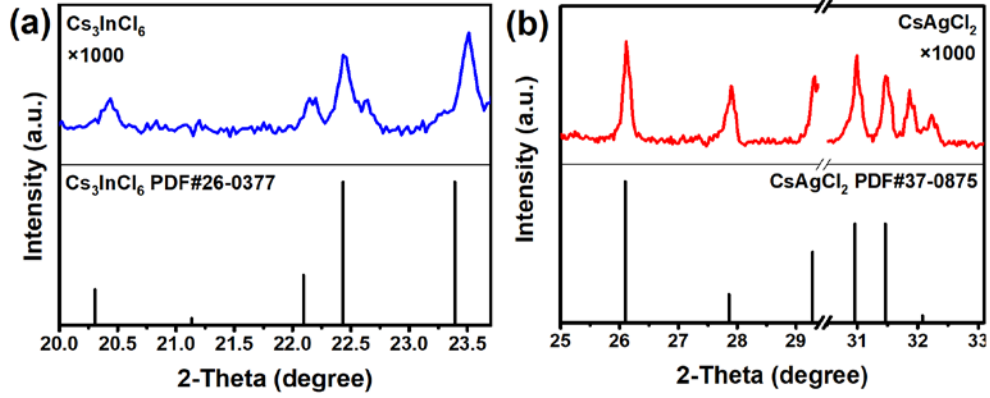


Fig. S1 The magnified images of the impurity (a) Cs_3InCl_6 and (b) CsAgCl_2 phases together with their reference patterns.

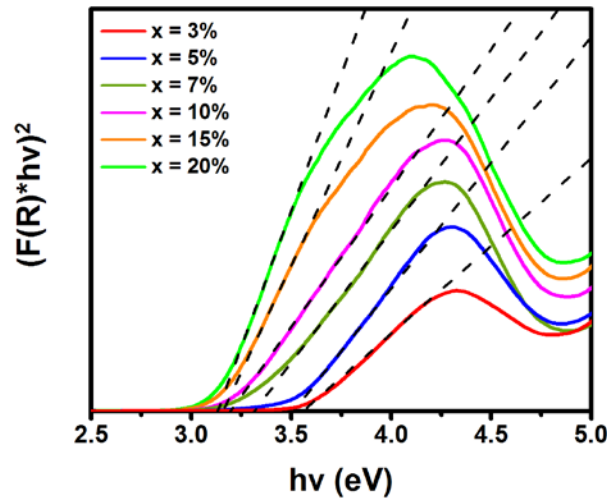


Fig. S2 The diffuse reflection (DR) spectra of $\text{Cs}_2\text{AgIn}_{1-x}\text{Cl}_6:x\text{Cr}^{3+}$ ($x = 0.03, 0.05, 0.07, 0.1, 0.15$ and 0.2) with $[F(R) \cdot hv]^2$ as a function of photon energy, for determining the band gap energy.

The optical band gap of $\text{Cs}_2\text{AgInCl}_6$ host can be estimated according to eqn. S1,¹

$$[F(R_\infty)hv]^n = A(hv - E_g) \quad (S1)$$

where hv is the photon energy; A is a proportional constant; E_g represents the value of the band gap; $n = 2$ since the $\text{Cs}_2\text{AgInCl}_6$ host absorption is a direct transition;² and $F(R_\infty)$ is the Kubelka-Munk function defined as,¹

$$F(R_\infty) = \frac{(1-R)^2}{2R} \quad (S2)$$

where R represents the reflection coefficient.

From the corresponding Tauc plot of $[F(R_\infty)hv]^2$ versus hv (Fig. S2), we can get the optical band gap of all the samples.

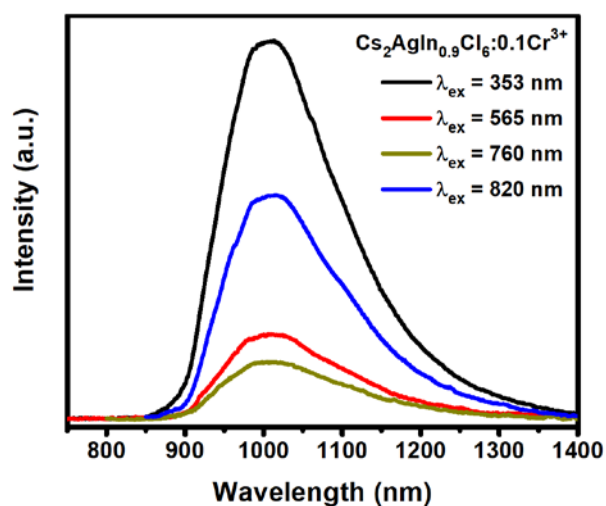


Fig. S3 PL spectra of $\text{Cs}_2\text{AgIn}_{0.9}\text{Cl}_6:0.1\text{Cr}^{3+}$ sample excited by 353, 565, 760 and 820 nm, respectively.

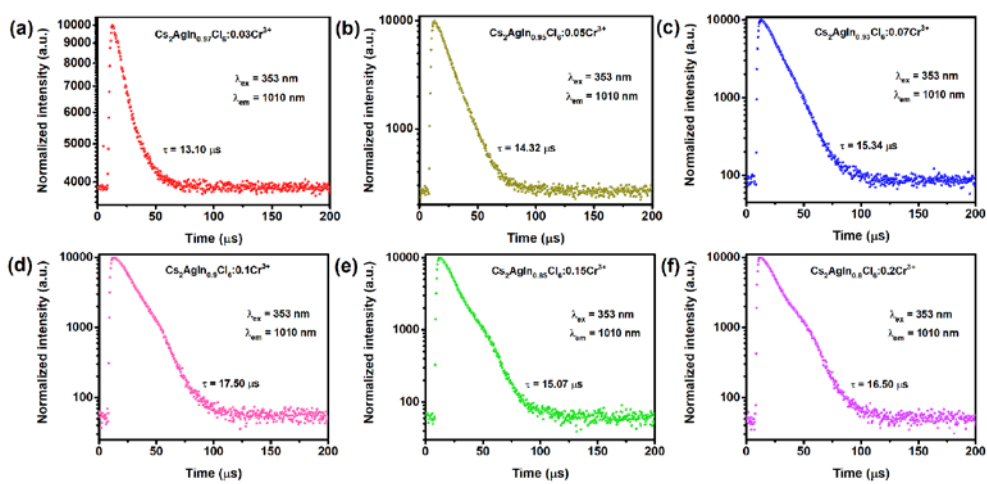


Fig. S4 (a-f) The RT decay curves of $\text{Cs}_2\text{AgIn}_{1-x}\text{Cl}_6:x\text{Cr}^{3+}$ ($x = 0.03, 0.05, 0.07, 0.1, 0.15$ and 0.2) excited by 353 nm monitoring at 1010 nm.

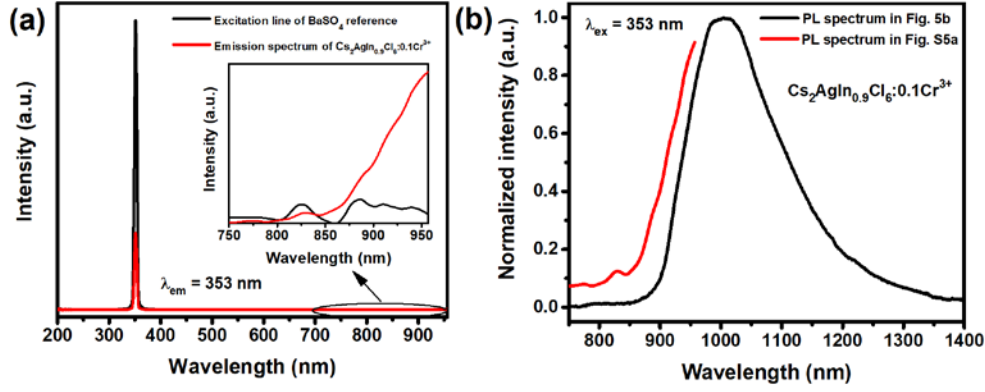


Fig. S5 (a) Excitation lines of BaSO₄ and Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺, and the emission spectrum of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor collected by using an integrating sphere. The inset shows the magnification of the emission spectrum of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺. (b) Normalized emission spectra of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor in Fig. 5b and Fig. S5a.

To determinate the PLQY values of the obtained Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor, the emission spectra of the sample and the reference material BaSO₄ were recorded under different excitation light ranging from 196 to 957 nm. In order to describe the calculation method clearly, we use 353 nm excitation source as an example to calculate the PLQY value as shown in Fig. S5. Due to limitations of the instrument, we can obtain the number of emitted photons, N_{em} , through the proportion of steady-state emission spectrum in the room temperature (RT) as given in eqn. S3,

$$\frac{\int_{750}^{957} I_{Sample_{Fig.5b}} d\lambda}{\int_{750}^{1400} I_{Sample_{Fig.5b}} d\lambda} = \frac{\int_{750}^{957} I_{Sample_{Fig.S5a}} d\lambda}{N_{em}} \quad (S3)$$

In eqn. S3, $\int_{750}^{957} I_{Sample_{Fig.5b}} d\lambda$, $\int_{750}^{1400} I_{Sample_{Fig.5b}} d\lambda$ and $\int_{750}^{957} I_{Sample_{Fig.S5a}} d\lambda$ represent the PL integrated intensities of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor at 750 to 957 nm, 750 to 1400 nm in Fig. 5b and 750 to 957 nm in Fig. S5a, respectively. And the values are 834266.5, 6231770 and 6181.13, respectively. Therefore, the number of emitted photons, N_{em} , is calculated to be 46171.55.

In addition, as shown in Fig. S5b, the shape of PL spectra in Fig. 5b and Fig. S5a are almost same demonstrating the accuracy of the calculation method according to eqn. S3.

By presuming a total reflection of the incident light which is equivalent to the PLQY value of the reference material BaSO₄, the PLQY of the obtained Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor can be derived from the following equation,³

$$PLQY = \frac{N_{em}}{N_{abs}} = \frac{N_{em}}{\int_{338}^{368} I_{BaSO_4} d\lambda - \int_{338}^{368} I_{Sample_{Fig.S5a}} d\lambda} \quad (S4)$$

In eqn. S4, $\int_{338}^{368} I_{BaSO_4} d\lambda$ and $\int_{338}^{368} I_{Sample_{Fig.S5a}} d\lambda$ represent the integrated intensities of BaSO₄ and Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor at 338 to 368 nm in Fig. S5a. And the values are 511759.63 and 137806.87, respectively. Therefore, the PLQY of the obtained Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ phosphor excited at 353 nm can be calculated to be 12.35%.

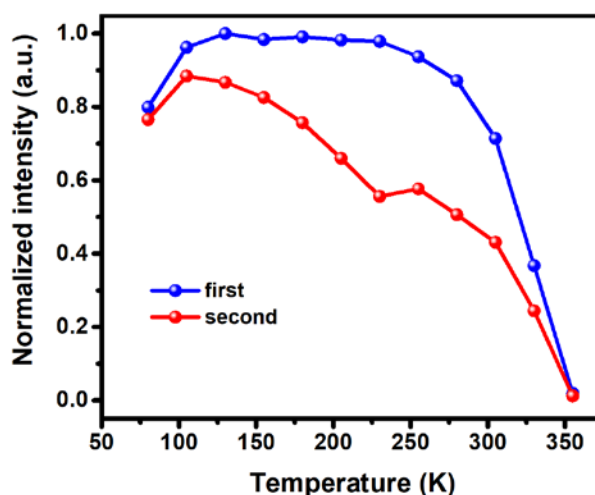


Fig. S6 The dependence of PL intensity of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ on heating temperature measured twice for the same sample.

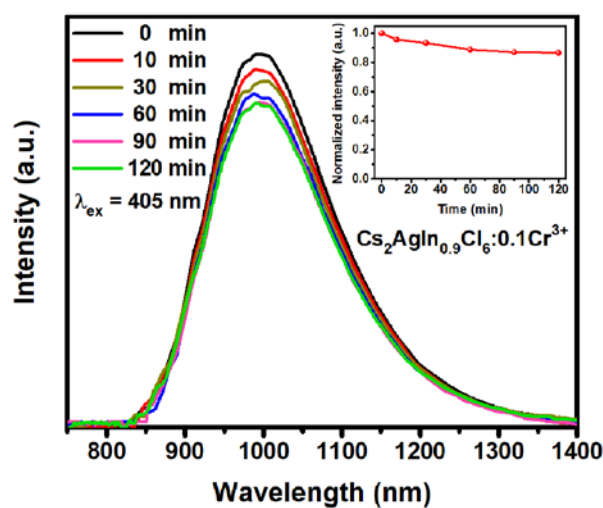


Fig. S7 PL spectra of Cs₂AgIn_{0.9}Cl₆:0.1Cr³⁺ exposed at 405 nm UV light for 0 minute, 10 minutes, 30 minutes, 60 minutes, 90 minutes and 120 minutes, and the inset shows the PL intensity dependence of irradiation time.

References

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- 2 J. Zhou, Z. G. Xia, M. S. Molokeev, X. W. Zhang, D. S. Peng and Q. L. Liu, *J. Mater. Chem. A*, 2017, **5**, 15031-15037.
- 3 S. Möller, A. Katelnikovas, M. Haase, T. Jüstel, *J. Lumin.*, 2016, **172**, 185-190.