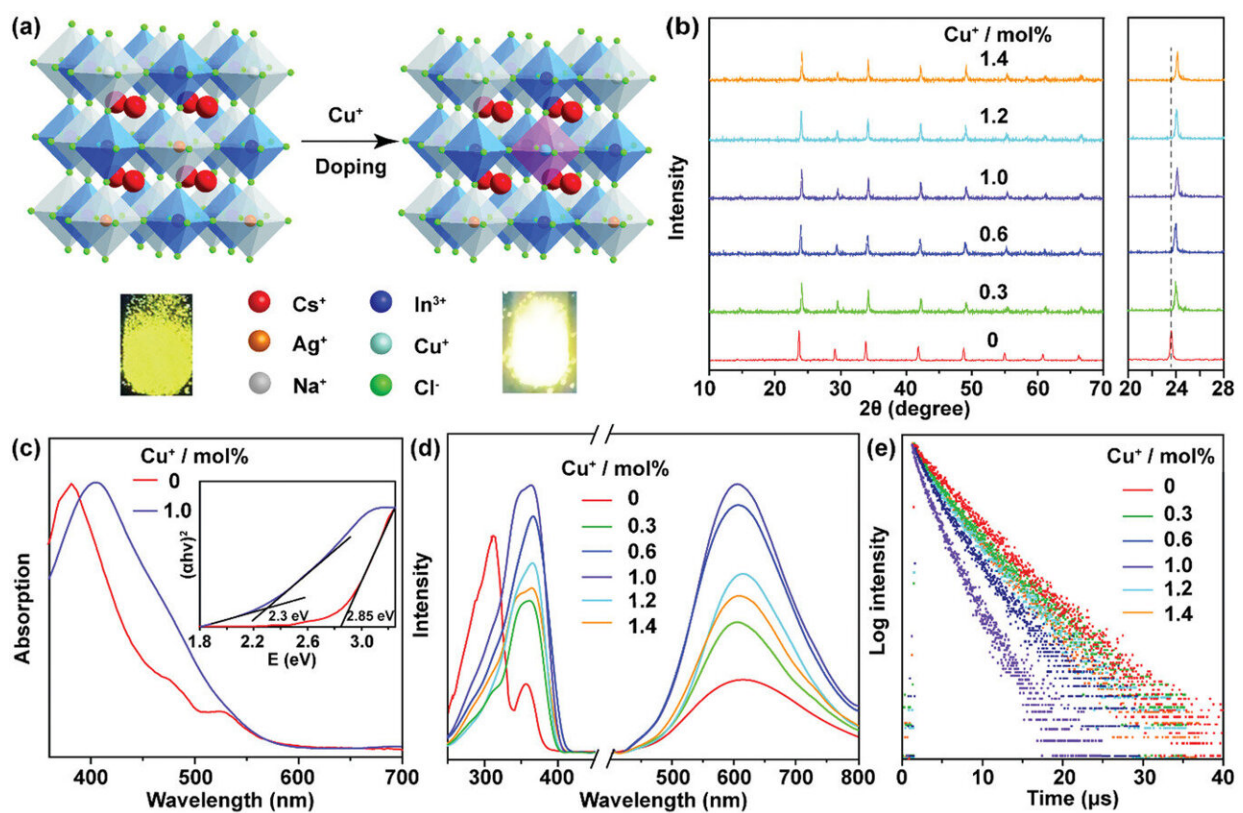


Cu⁺ doping enhances self-trapped exciton emission in alloyed Cs₂(Ag/Na)InCl₆ double perovskite

March 28 2022, by Liu Jia



a) Crystal structure of Cs₂(Ag/Na)InCl₆ and the crystallographic site for Cu⁺ dopants. The PL photographs ($\lambda_{\text{ex}} = 365 \text{ nm}$) for Cs₂(Ag/Na)InCl₆ and Cs₂(Ag/Na)InCl₆: 1.0%Cu⁺ powders are presented, showing significantly enhanced PL of the crystals upon Cu⁺ doping. b) Powder XRD patterns of Cs₂(Ag/Na)InCl₆: x%Cu⁺ with different Cu⁺ doping concentrations. The enlarged 2 θ range (20–28°) of XRD patterns shows a monotonic shift of the diffraction peaks to higher angle with increasing the Cu⁺ concentration. c)

Optical absorption spectra of $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6$ and $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6: 1.0\%\text{Cu}^+$. The inset shows the corresponding Tauc plots of the absorption spectra. d) PL excitation spectra ($\lambda_{\text{em}} = 605 \text{ nm}$), PL emission spectra ($\lambda_{\text{ex}} = 365 \text{ nm}$), and e) PL decay curves ($\lambda_{\text{em}} = 605 \text{ nm}$) of $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6: x\%\text{Cu}^+$ with different Cu^+ doping concentrations. Credit: *Advanced Science* (2022). DOI: 10.1002/advs.202103724

All-inorganic 3D lead-free double perovskites (DPs) with broadband self-trapped exciton (STE) emission have shown great promise as alternatives to lead halide perovskites in various optoelectronic applications such as light-emitting diodes (LEDs) and photodetectors. A fundamental understanding of the effect of doping on the optical properties of DPs, especially the STE dynamics, is of vital importance for their performance optimization and applications.

In a study published in *Advanced Science*, the research group led by Prof. Chen Xueyuan from Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences developed a unique strategy via Cu^+ doping to achieve efficient STE [emission](#) in the alloyed lead-free $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6$ DP crystals.

This unique strategy based on Cu^+ doping boosts the STE emission in the alloyed $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6$ DPs. The researchers used a small amount (1.0 mol%) of Cu^+ doping to realize the boosted STE emission in the crystals, with photoluminescence (PL) quantum yield increasing from 19.0% to 62.6% and excitation band shifting from 310 nm to 365 nm.

They comprehensively surveyed the effect of Cu^+ doping on the [electronic structure](#) and optical properties of $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6$ and the STE dynamics. The as-synthesized $\text{Cs}_2(\text{Ag/Na})\text{InCl}_6: \text{Cu}^+$ crystals exhibit significantly enhanced PL stemming from the increased radiative

recombination rate of STEs as well as the improved STE density.

By means of temperature-dependent PL and ultrafast femtosecond transient absorption spectroscopies, the researchers unraveled that the remarkable PL enhancement was ascribed to the increased density and radiative recombination rate of STEs, as a result of symmetry breakdown of the STE wavefunction at the octahedral Ag^+ site induced by Cu^+ [doping](#).

Besides, the researchers demonstrated the excellent air, structural and [thermal stability](#) of these Cu^+ -doped $\text{Cs}_2(\text{Ag}/\text{Na})\text{InCl}_6$ crystals, and revealed their great potentials as efficient yellow-emitting phosphors for application in near-ultraviolet (NUV)-converted white LEDs.

This study provides deep insights into the STE dynamics in Cu^+ -doped $\text{Cs}_2(\text{Ag}/\text{Na})\text{InCl}_6$, thereby laying a foundation for future design of new lead-free DPs with efficient STE emission.

More information: Xingwen Cheng et al, Boosting the Self-Trapped Exciton Emission in Alloyed $\text{Cs}_2(\text{Ag}/\text{Na})\text{InCl}_6$ Double Perovskite via Cu^+ Doping, *Advanced Science* (2022). [DOI: 10.1002/advs.202103724](https://doi.org/10.1002/advs.202103724)

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