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

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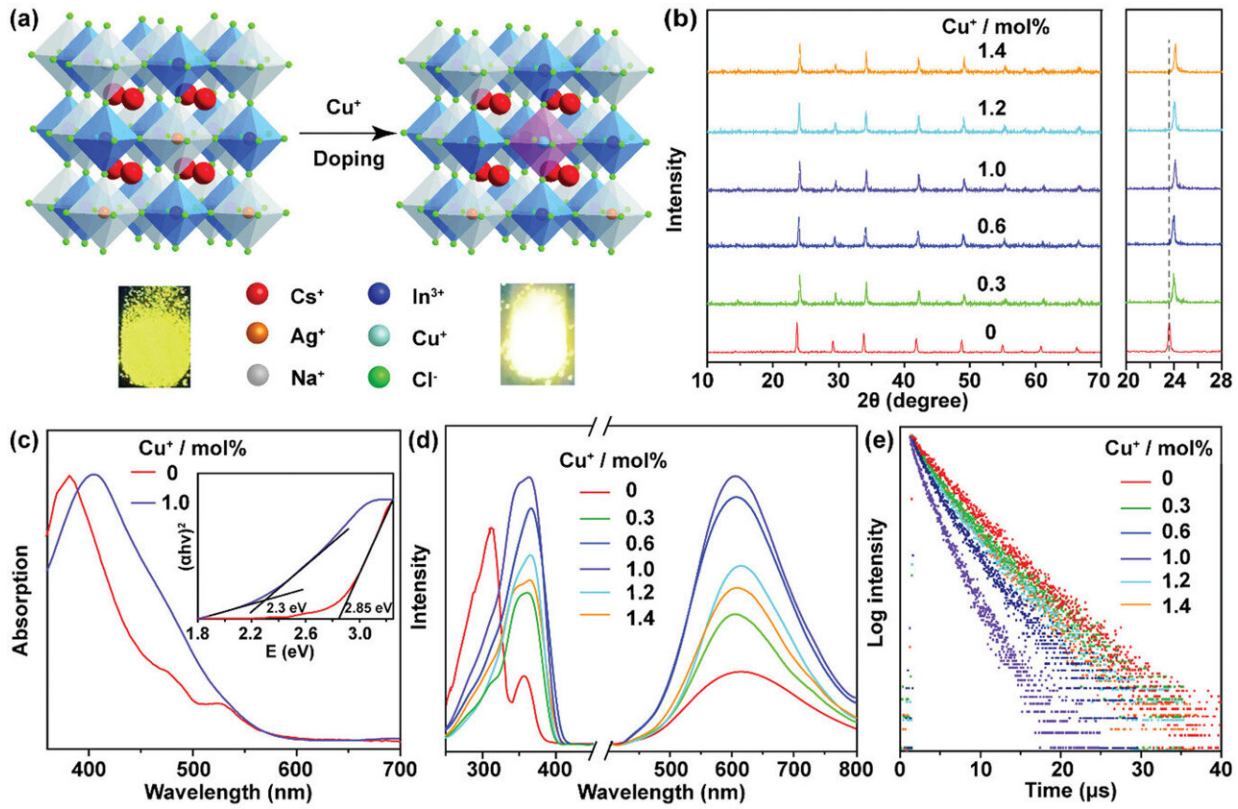

a) Crystal structure of $Cs_2(Ag/Na)InCl_6$ and the crystallographic site for Cu^+ dopants. The PL photographs (λ_{ex} = 365 nm) for $Cs_2(Ag/Na)InCl_6$ and $Cs_2(Ag/Na)InCl_6$: 1.0%Cu^+ powders are presented, showing significantly enhanced PL of the crystals upon Cu^+ doping. b) Powder XRD patterns of $Cs_2(Ag/Na)InCl_6$: x%Cu^+ with different Cu^+ doping concentrations. The enlarged 2θ 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 $Cs_2(Ag/Na)InCl_6$ and $Cs_2(Ag/Na)InCl_6$: 1.0%Cu^+. The inset shows the corresponding Tauc plots of the absorption spectra. d) PL excitation spectra (λ_{em} = 605 nm), PL emission spectra (λ_{ex} = 365 nm), and e) PL decay curves (λ_{em} = 605 nm) of $Cs_2(Ag/Na)InCl_6$: x%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 $Cs_2(Ag/Na)InCl_6$ DP crystals.

This unique strategy based on Cu^+ doping boosts the STE emission in the alloyed $Cs_2(Ag/Na)InCl_6$ 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 $Cs_2(Ag/Na)InCl_6$ and the STE dynamics. The as-synthesized $Cs_2(Ag/Na)InCl_6$: 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 $Cs_2(Ag/Na)InCl_6$ 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 $Cs_2(Ag/Na)InCl_6$, 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 Cs 2 (Ag/Na)InCl 6 Double Perovskite via Cu + Doping, *Advanced Science* (2022). DOI: 10.1002/advs.202103724

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