Modification of Bandgap for Lead-Free Double Perovskite $Cs_2AgInCl_6$ with Bi Doping

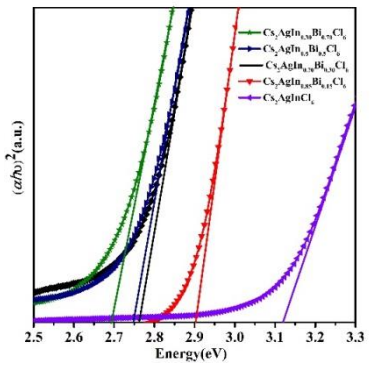
Hassan Siddique, Da Huang, Xiangqi Wang, Rucheng Dai, Zhongping Wang, Zejun Ding, and Zengming Zhang*

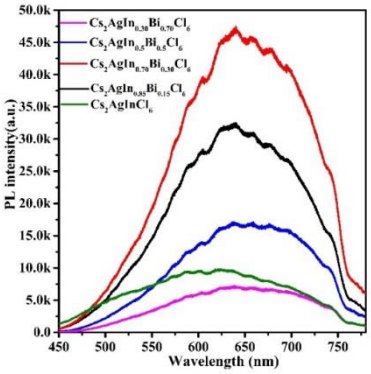
University of Science and Technology of China, Hefei 230026, China;

*Corresponding author: zzm@ustc.edu.cn

Abstract

Lead halide perovskites have the excellent luminescent properties but exist some vital disadvantages such as instability and Pb toxicity. Lead-free double perovskites draw attention due to a possible candidate for environment-friendly materials. Direct bandgap lead-free halide of $Cs_2AgInCl_6$ is one of them. [1] In this work Bi doping $Cs_2AgInCl_6$ (CAIC) was successfully prepared. Bi dopant above 15% CAIC can restrict the parity forbidden transition responding to sub absorption peak around 600 nm.[2] On the other hand, the intensity of photoluminescence enhances with the increasing Bi dopant and touches the maximum around 30% doping, then gradually loses its intensity with further doping due to the mechanism of the concentration quenching at room temperature. Bi doping in CAIC can also modify the band gap. The absorption spectra indicate that the band gap reduces from 3.10eV without Bi doping to 2.68eV for $Cs_2AgIn_{0.30}$ $Bi_{0.70}Cl_6$. PL decay life time reveals the good intrinsic excitonic feature with less defect trappers [3]. Average life time for $Cs_2AgIn_{0.70}$ $Bi_{0.30}Cl_6$ is 490 ns which is least among all other $Cs_2AgIn_{(1-x)}Bi_xCl_6$ doping. Thermogravimetric analysis (TGA) result reveals thermal stability of $Cs_2AgIn_{0.30}$ $Bi_{0.70}Cl_6$ for the high-temperature 506ºC. The Bi doping can decrease the band gap, restrict defect states, enhance PL and improve stability; these good performances make $Cs_2AgIn_{(1-x)}Bi_xCl_6$ more suitable for optoelectronic properties.





References

1. Volonakis *et al*, J. Phys. Chem. Lett. 8, 772−778 (2017).
2. Luo *et al*, ACS Photonics. 5, 398−405 (2018).
3. Zhang *et al.* ACS Nano. 9, 4533–4542 (2015) .