Tunable Luminescence by B-site Substitution in $Cs_2NaInCl_6$

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A series of double halide perovskites (DHPs) with the general composition $Cs_2Ag_{0.2}Na_{0.4}In_{0.6}X_{0.4}Cl_6$ (X = Si, Ti, Zr) was synthesized and characterized, including studies of photoluminescence (PL), temperature-dependent photoluminescence excitation (PLE), and luminescence kinetics. The materials were synthesized via a hydrothermal method. The phase purity and elemental composition of the synthesized perovskites were confirmed by X-ray diffraction (XRD) and scanning electron microscopy (SEM), equipped with energy-dispersive X-ray spectroscopy (EDS), which demonstrated that the samples corresponded to the specified stoichiometry. The PL spectra exhibit a systematic shift toward the lower-energy region with substitution from Si to Zr, correlating with the progressive increase in the ionic radii of the substituting cations. All samples display broad, asymmetric emission bands, characteristic to self-trapped excitonic (STE) states. Temperature-dependent PL measurements reveal a gradual decrease in emission intensity with increasing temperature for all samples. The maximum emission intensity is observed in the range of 160–200 K, corresponding to optimal conditions for radiative recombination, whereas the lowest intensity is recorded at 80–100 K, where radiative centers are effectively frozen. An increase in temperature is accompanied by a red shift of the PL bands across all compositions. In the Ti-doped DHP, a pronounced blue shift at low temperatures is observed, which can be attributed to the involvement of $Ti4^{+}$–related electronic states. An analysis of the activation energy of thermal luminescence quenching and the results of time-resolved spectroscopy revealed the activation of thermal processes in the titanium-containing sample and their rapid decay, whereas replacing titanium with silicon leads to more stable luminescence in the crystal under study. Thus, the enhanced luminescence characteristics of double-halide perovskites doped with Ti, Si, and Zr highlight their potential for advanced photonic and optoelectronic applications.

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