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# Cu-Based Chalcogenide Nanocrystals $Cu_2ZnA(S_xSe_{4-x})$ (A = Al, Ga, In): Synthesis, Characterization, and S–Se Alloying Effects

We report a new class of Cu-based chalcogenide nanocrystals, $Cu_2ZnAS_xSe_{4-x}$, (A= Al, Ga, In), synthesized via a novel modified hot-injection route. The nanocrystals were experimentally characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-vis absorbance spectroscopy, and steady-state and time-resolved photoluminescence (PL). Analysis of XRD peak intensities showed that all compositions crystallize into pure wurtzite phase (space group: P63mc, no. 186). Scherrer analysis of the peak broadening observed in the diffraction pattern showed nanocrystal sizes ranging from 2.7 ± 0.9 to 11.2 ± 0.8 nm, consistent with TEM imaging. These materials exhibit a direct band gap with strong absorption in the visible range, making them promising candidates for solar spectrum harvesting in photovoltaics. Optical absorption measurements and Tauc plot analyses yielded estimated bandgaps between 2.2 and 3.0 eV. S-Se alloying allows for fine tuning of bandgaps through selenium concentration, with higher selenium content correlating with larger crystallite size and lower bandgap. Theoretical calculations using density functional theory within the virtual crystal approximation also support these observations. PL characterization showed a broad fluorescence spectrum with a peak located in the violet spectral region, around 435 nm (2.85 eV). This energy is close to the estimated direct bandgap value, suggesting emission from direct inter-band transitions. Time-Resolved Photoluminescence (TRPL) showed similar lifetimes across all samples, varying between 2.0 and 2.5 ns, when fitted with a single exponential decay model. The similarity of the TRPL lifetime data suggests a common trapping mechanism that dominated the recombination processes in all the samples, most likely hole trapping. In summary, these new materials exhibit tunable optoelectronic properties, making them promising for photovoltaics and light-harvesting applications requiring absorption in the visible range.

## Topical Area

Hard matter: energy materials

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