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Synthesis of Shape-Controlled Wurtzite $CuIn_xGa_{1-x}S_2$ Nanocrystals with Tunable Band Gap

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$CuIn_xGa_{1-x}S_2$ is a promising material for high efficiency solar cells because of its high absorption coefficient, direct band gap, and low toxicity. Colloidal $CuIn_xGa_{1-x}S_2$ nanocrystals (NCs) can be used to deposit films by spin-casting, doctor-blading, screen printing, or dip-coating for low-cost fabrication of solar cells. In addition, since the In and Ga atoms are randomly distributed at the cation sites, the wurtzite phase offers flexibility of stoichiometry control.

We have synthesized shape controlled monodisperse wurtzite phase $CuIn_xGa_{1-x}S_2$ (CIGS) nanocrystals (NCs) over the whole composition range by using a facile solution-based method. A systematic shift in the x-ray diffraction peaks to higher angles is observed for the NCs with increasing gallium substitution, as is expected because of the smaller size of galium ion as compared to indium. The morphology of the monodisperse CIGS NCs can be tuned from bullet-like to tadpole-like shapes using oleylamine and 1-octadecene as solvents, respectively. The composition of the NCs, as determined by atomic absorption spectroscopy, match very well with the expected ratio, demonstrating precise stoichiometry control of the ternary and quaternary CIGS NCs. The band gap of the NCs increases linearly with increasing Ga concentration, with values ranging between 1.53 to 2.48 eV. These values are close to the reported values (1.53 to 2.43 eV) for the chalcopyrite phase. Colloidal suspensions of the nanocrystals are attractive for use as inks for low-cost fabrication of thin film solar cells by spin or spray coating.