Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Nanocluster seed-mediated synthesis of $CuInS_2$ quantum dots, nanodisks, nanorods, and doped Zn-Ga-$CuInS_2$ quantum dots

Sanjaya D. Perera, Haitao Zhang, Xiaoyue Ding, Andrew Nelson, Richard D. Robinson

Cornell University, Department of Materials Science and Engineering, 214 Bard Hall, Ithaca, New York 14853, United States

Supporting Information

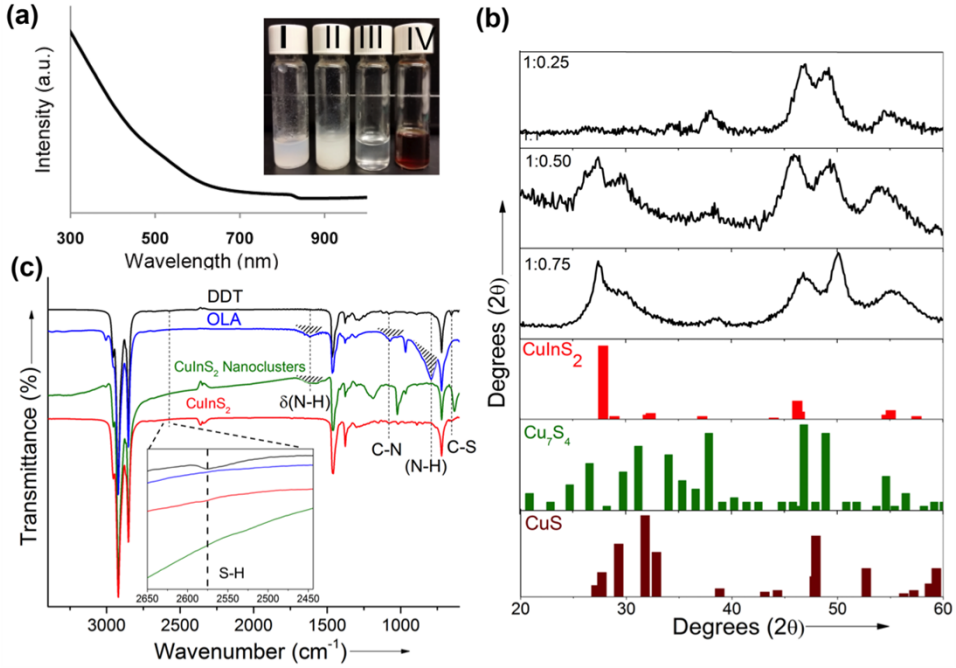

Figure s1. a) UV-vis optical absorption spectrum of $CuInS_2$ nanoclusters. Inset image shows a photograph of the following compounds in dodecanethiol (DDT) at room temperature: I) CuCl, II) $InCl_3$, III) a mixture of Cu and In (1:1 molar ratio) and IV) $CuInS_2$ nanoclusters. b) XRD patterns for products obtained during the nanocluster formation stage with different Cu:In molar ratios. Increasing the molar ratio of Cu:In to 1:0.75 favors the formation of $CuInS_2$, while lower molar ratios result mixtures of Cu_7S_4 and CuS. c) FT-IR spectra of DDT, oleylamine (OLA), $CuInS_2$ nanoclusters and $CuInS_2$ nanoparticles. Inset image shows the weak S-H vibrations corresponding to DDT, which are present in pure DDT and in the nanoclusters. The absence of S-H vibrations in both clusters and the final $CuInS_2$ nanoparticles indicates the capping of $CuInS_2$ by DDT.

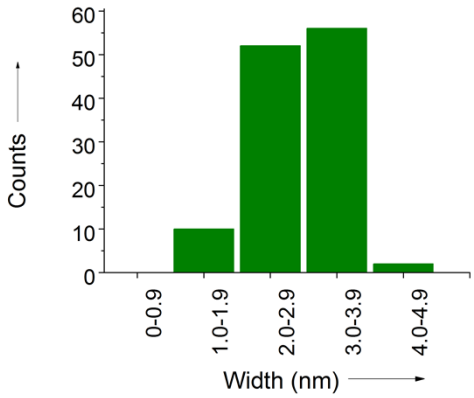

Figure s2. Distribution of the thickness of nanodisks.

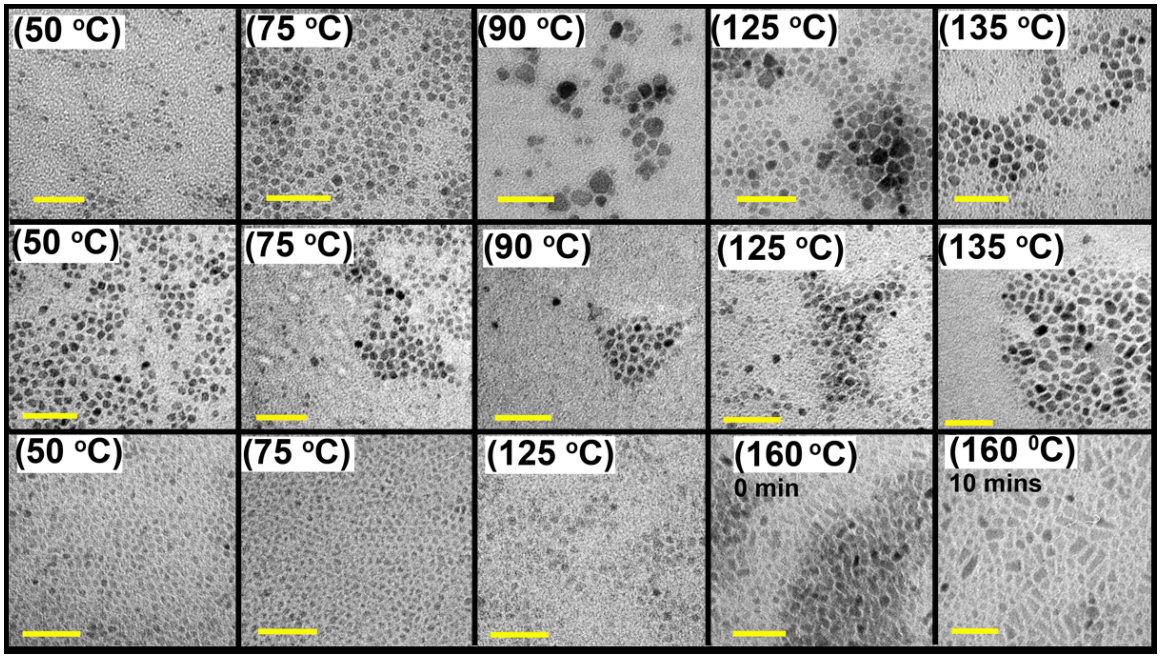

Figure s3. Aliquots of $CuInS_2$ q-dots (first row), nanodisks (second row), nanorods (third row) collected at different temperatures.

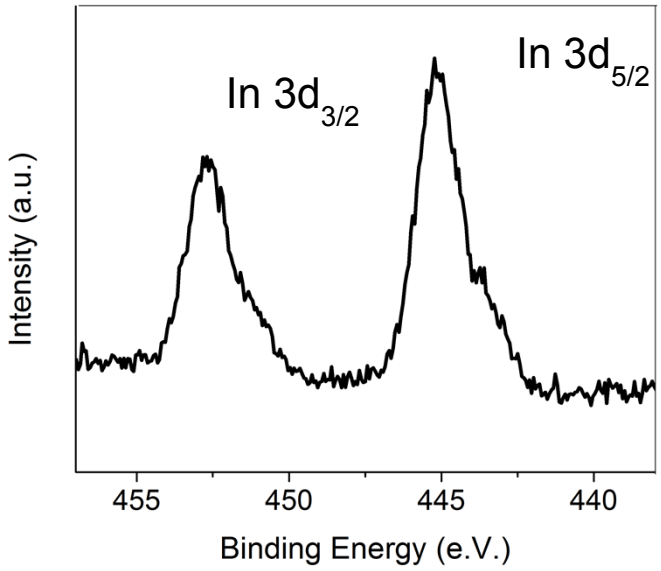

Figure s4. XPS spectra of In 3d core electrons in CuInZnS.

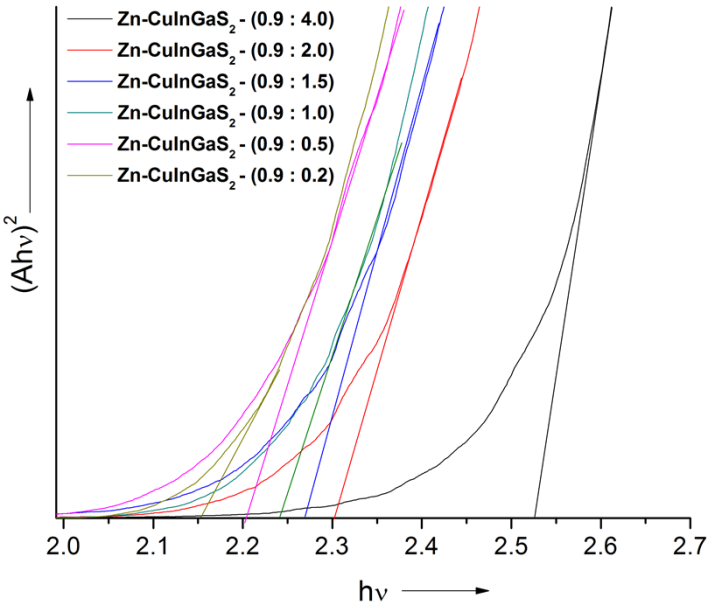

Figure s5. Least-squares fit of the linear region of the optical absorption edge corresponding to different Ga/Cu starting molar ratios. (A - absorbance, h - Planck's constant, ν -frequency).

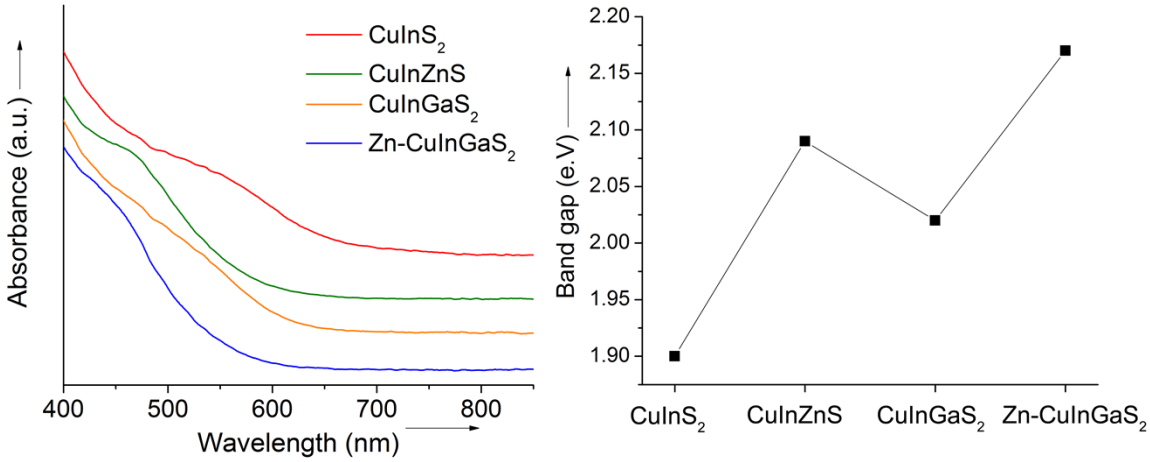

Figure s6. a) Comparison of optical absorption spectra of $CuInS_2$, CuInZnS, $CuInGaS_2$ and Zn-$CuInGaS_2$, which shows the synergistic effect of cation combination on the absorption edge. b) Synergistic effect of Zn and Ga on band gap. The differences in the band gaps of $CuInS_2$, CuInZnS, $CuInGaS_2$ and Zn-$CuInGaS_2$ clearly show the overall effect of incorporation of both Ga and Zn.