Supporting Information Available

Alloyed Semiconductor Nanocrystals with Broad Tunable Band Gaps

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Experimental section

I. Chemicals

$CuCl_2{\cdot}2H_2O$, $InCl_3{\cdot}4H_2O$, oleic acid (OA, 90%), oleylamine (OM, 70%), 1-dodecanethiol (DDT, 98%), 1-octadecene (ODE, 90%), sodium diethyl dithiocarbamate (Na-dedc) (NaS_2CNEt_2) (98%), $Zn(dedc)_2$ (98%), and ethanol (99.9%) were purchased from Aldrich.

II. Synthesis of $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals by a hot-injection approach

$Cu(dedc)_2$ and $In(dedc)_3$ were synthesized through the reactions of metal chloride with Na-dedc in water at room temperature. Complete details were described elsewhere.[1] A typical procedure for the synthesis of cubic $(CuInS_2)_{0.5}(ZnS)_{0.5}$ nanocrystals is as follows. 18.1 mg (0.05 mmol) of $Zn(dedc)_2$, 18.0 mg (0.05 mmol) of $Cu(dedc)_2$, 28.0 mg (0.05 mmol) of $In(dedc)_3$, 0.5 g of oleic acid, and 4.5 g of ODE were putted into a 50 mL three-neck flask. The mixture was heated to 200^{o}C under nitrogen flow. Then 0.5 mL of oleylamine was injected into the flask, and the temperature was kept at 200^{o}C for 2 min. Copious amount of ethanol was added to completely precipitation of nanocrystals. Hexagonal $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals were synthesized by the same procedure except that 0.5g of dodecanethiol was used in place of 0.5 g of oleic acid.

III. Characterization

UV-vis absorption spectra were recorded on a Shimadzu UV-1700 spectrometer with a resolution of 1.0 nm. The powder XRD patterns were recorded using a Panalytical X'Pert Pro X-ray diffractometer. TEM image was taken on a CM-120 electron microscope with an accelerating voltage of 120 kV. Energy Disperse Spectroscopy (EDS) spectrum was obtained by using a scanning electron microscope (JEOL JSM-6700F).

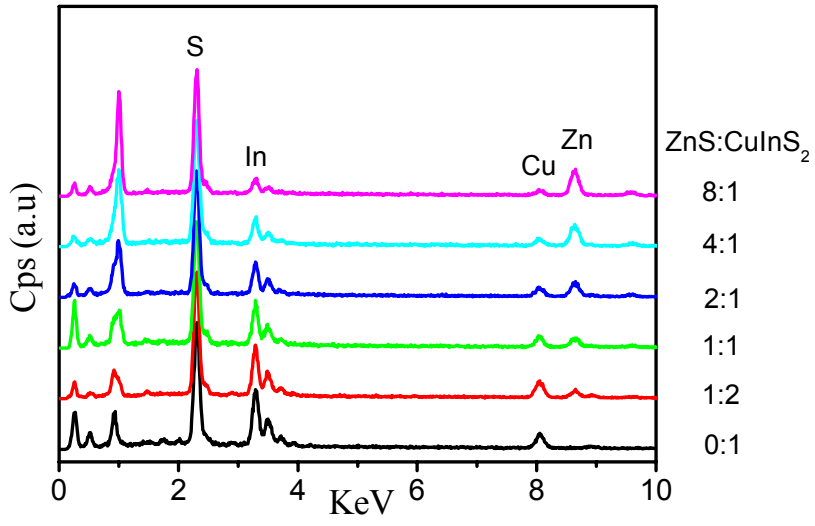

Figure S1 Energy Dispersive X-ray (EDX) spectra of cubic $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals.

Phase	Zn%	Cu%	In%	S%	ZnS/$CuInS_2$
Cubic	37.09	5.05	5.44	51.61	8:1
Cubic	32.29	8.25	8.89	50.57	4:1
Cubic	22.97	10.93	12.81	53.29	2:1
Cubic	15.88	14.18	16.70	53.23	1:1
Cubic	10.99	20.21	19.17	49.63	1:2
Cubic	------	24.93	23.05	50.64	0:1

Table S1 Composition determined by EDX spectra of cubic $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals and precursor ratios.

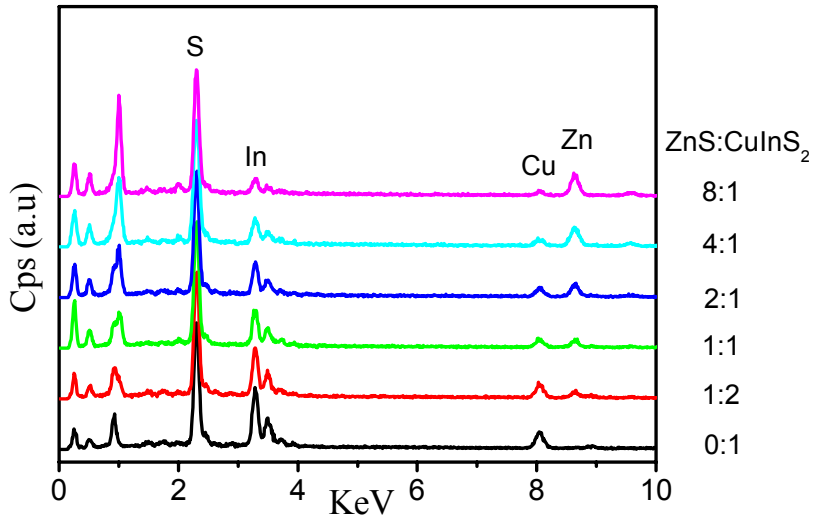

Figure S2 Energy Dispersive X-ray (EDX) spectra of hexagonal $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals.

Phase	**Zn%**	**Cu%**	**In%**	**S%**	**ZnS/CuInS$_2$**
Hexagonal	34.12	5.33	5.97	54.58	8:1
Hexagonal	28.64	8.02	9.97	53.57	4:1
Hexagonal	21.72	11.85	13.89	52.54	2:1
Hexagonal	14.14	13.39	17.84	54.63	1:1
Hexagonal	10.09	17.68	20.35	51.87	1:2
Hexagonal	------	22.52	24.02	51.93	0:1

Table S2 Composition determined by EDX spectra of hexagonal $(CuInS_2)_x(ZnS)_{1-x}$ nanocrystals and precursor ratios.

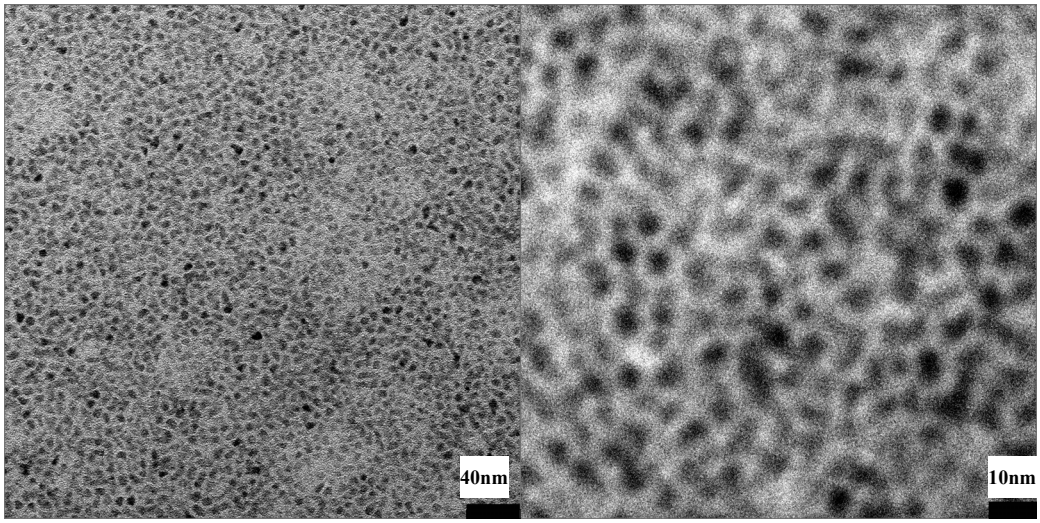

Figure S3 TEM images of hexagonal $(ZnS)_0(CuInS_2)_{1.0}$ nanocrystals.

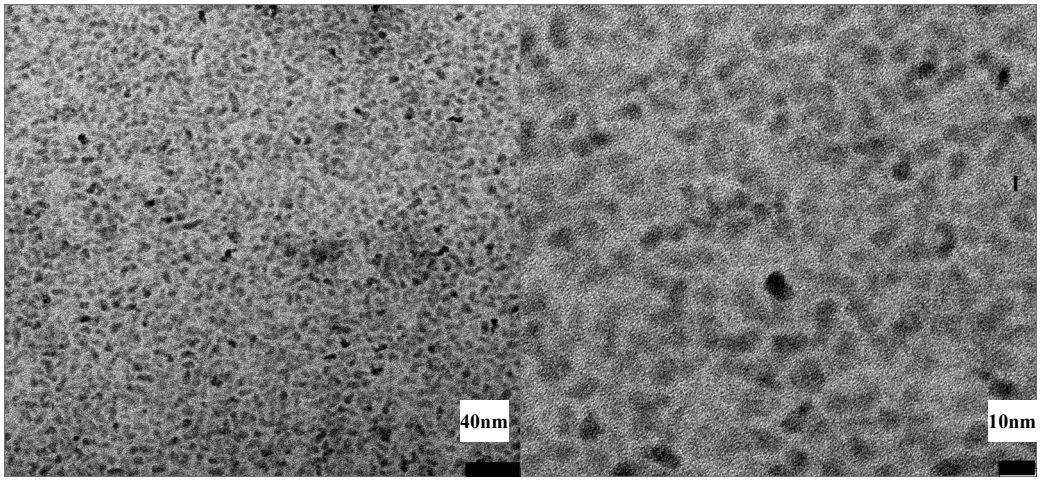

Figure S4 TEM images of hexagonal $(ZnS)_{0.33}(CuInS_2)_{0.66}$ nanocrystals.

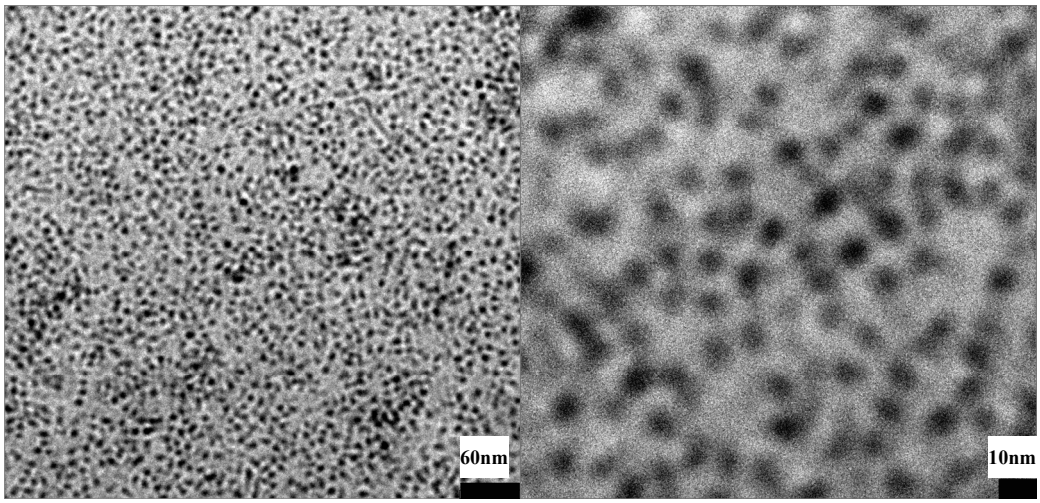

Figure S5 TEM images of hexagonal $(ZnS)_{0.66}(CuInS_2)_{0.33}$ nanocrystals.

(1) Pan, D.; An, L.; Sun, Z.; Hou, W.; Yang, Y.; Yang, Z.; Lu, Y. *J. Am. Chem. Soc.* **2008**, *130*, 5620.