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Supporting Information

Comparisons of the Structural and Optical Properties of o-$AgInS_2$, t-$AgInS_2$, and c-$AgIn_5S_8$ Nanocrystals and their Solid-Solution Nanocrystals with ZnS

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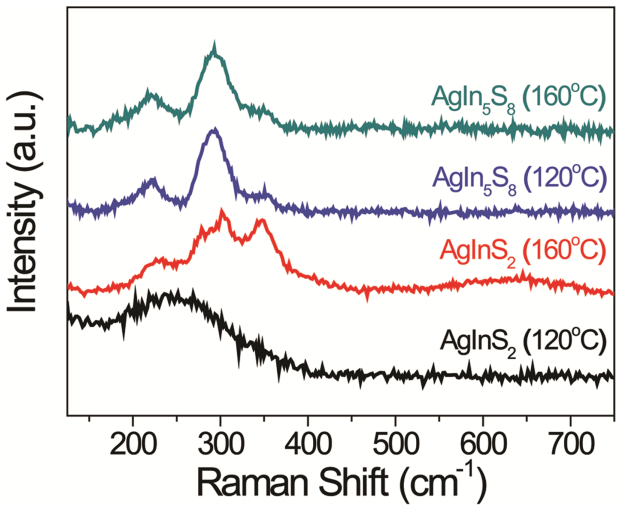

Fig. S1† Raman spectra of $AgInS_2$ and $AgIn_5S_8$ core NCs prepared at different temperatures.

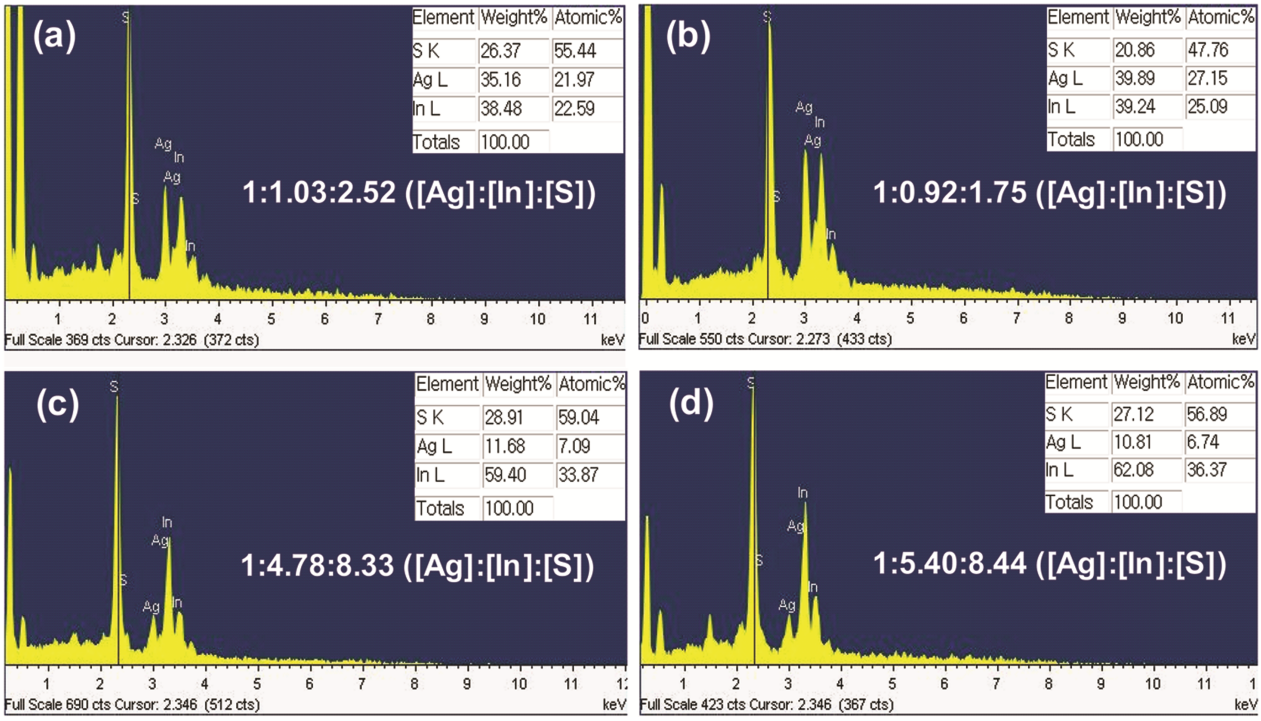

Fig. S2† EDS analysis of (a) o-$AgInS_2$ (120 ℃), (b) t-$AgInS_2$ (160 ℃), (c) c-$AgIn_5S_8$ (120 ℃) and (d) c-$AgIn_5S_8$ (160 ℃) core NCs.

Table S1† ICP-AES (for measuring the In contents), AAS (Ag) and EA (S) analysis of o-$AgInS_2$ (120 ℃), t-$AgInS_2$ (160 ℃), c-$AgIn_5S_8$ (120 ℃) and c-$AgIn_5S_8$ (160 ℃) core NCs.

	Weight %			Atomic %			[Ag]:[In]:[S]
	Ag	In	S	Ag	In	S	
o-$AgInS_2$ (120 ℃)	28.2	28.7	17.8	24.5	23.4	52.1	1:0.96:2.13
t-$AgInS_2$ (160 ℃)	29.2	27.7	16.2	26.6	23.7	49.7	1:0.89:1.87
c-$AgIn_5S_8$ (120 ℃)	7.67	41.0	18.0	7.20	36.1	56.7	1:5.01:7.88
c-$AgIn_5S_8$ (160 ℃)	5.99	35.1	15.2	6.60	36.6	56.8	1:5.46:8.46

Table S2† Summary of the average sizes measured from TEM images of the o-$AgInS_2$ (120 ℃), t-$AgInS_2$ (160 ℃) and c-$AgIn_5S_8$ (120 and 160 ℃) NCs.

(℃)	120		160	
	o-$AgInS_2$	c-$AgIn_5S_8$	t-$AgInS_2$	c-$AgIn_5S_8$
Average size, a (nm)	2.58	2.50	3.27	3.15
Average size, b (nm)	2.80	2.75	3.54	3.50

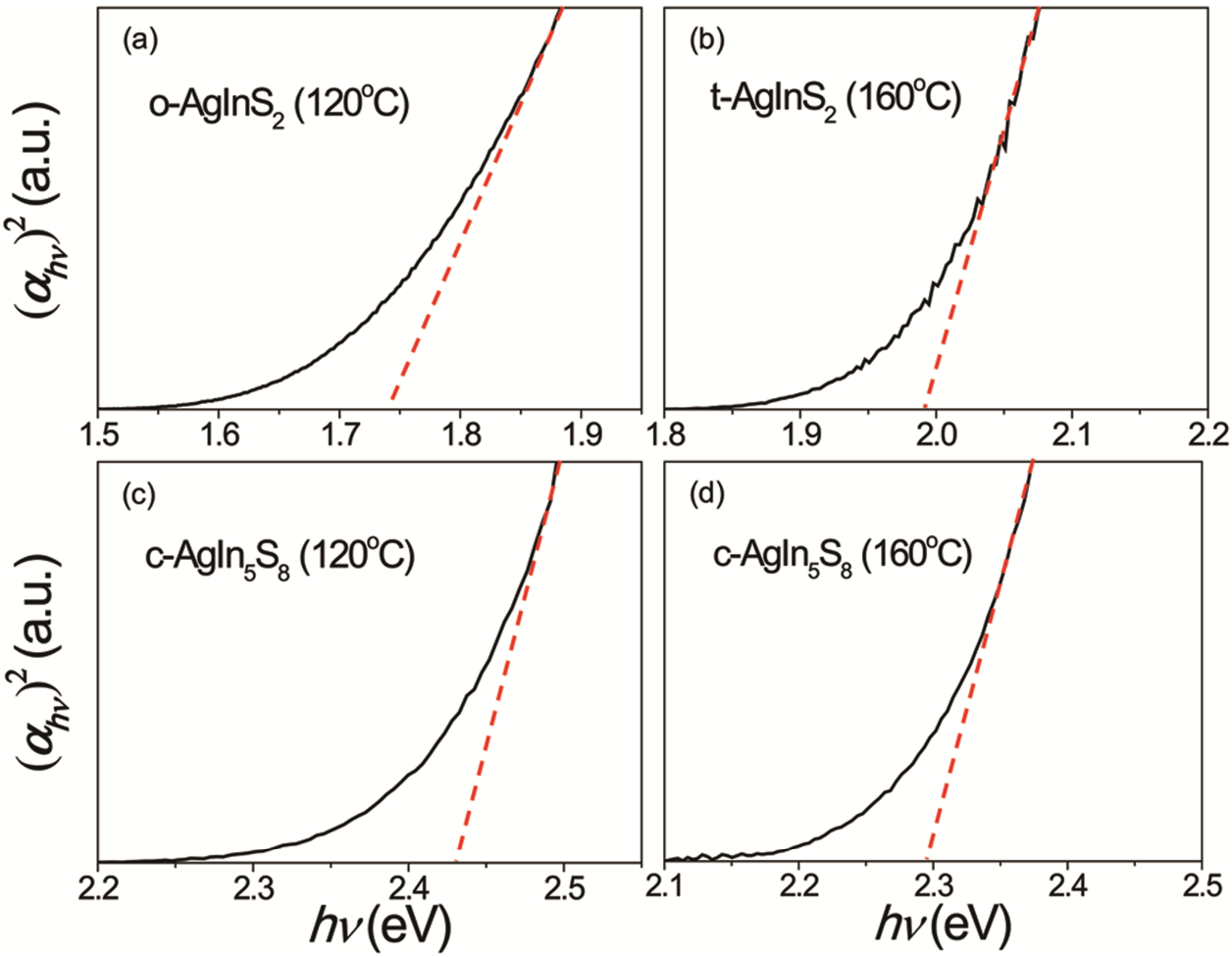

Fig. S3† The calculation of the optical band gaps of (a) o-$AgInS_2$ (120 ℃), (b) t-$AgInS_2$ (160 ℃), (c) c-$AgIn_5S_8$ (120 ℃), and (d) c-$AgIn_5S_8$ (160 ℃) after extrapolating the linear portion of the plot of $(\alpha_{h\nu})^2$ vs $h\nu$.

Table S3† Summary of the average sizes measured from TEM images of the o-$AgInS_2$/ZnS (120-120 ℃), t-$AgInS_2$/ZnS (160-160 ℃) and c-$AgIn_5S_8$/ZnS (120-120 and 160-160 ℃) alloyed NCs.

(℃)	120-120		160-160	
	o-$AgInS_2$	c-$AgIn_5S_8$	t-$AgInS_2$	c-$AgIn_5S_8$
Average size, a (nm)	3.13	2.82	3.55	3.38
Average size, b (nm)	3.18	3.05	3.80	3.68

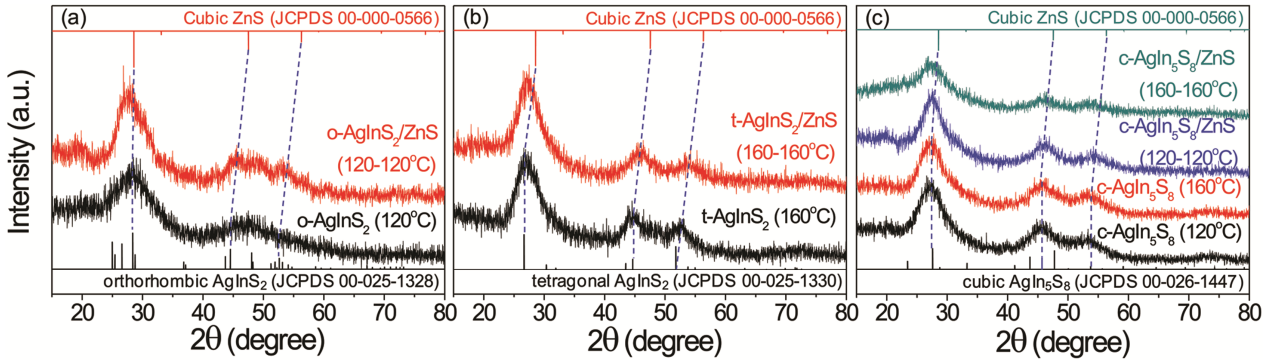

Fig. S4† XRD patterns showing each solid-solution of (a) o-$AgInS_2$/ZnS (120-120 ℃), (b) t-$AgInS_2$/ZnS (160-160 ℃) and (c) c-$AgIn_5S_8$/ZnS (120-120 and 160-160 ℃) alloyed NCs.

Table S4† Summary of core reaction temperatures, second preparation temperatures, calculated optical band gaps, CIE color coordinates, PL peaks, FWHMs and QY values for the four different NC samples.

	Core Reaction Temperature (℃)	Second Preparation Temperature (℃)	Optical Bandgap, E_g (eV)	CIE x	CIE y	PL Peak Wavelength (nm)	FWHM (nm)	Quantum Yield (%)
o-$AgInS_2$/ZnS	120	180	2.34	0.52	0.47	577	105	42.9
t-$AgInS_2$/ZnS	160	180	2.25	0.52	0.46	570	147	24.9
c-$AgIn_5S_8$/ZnS	120	180	2.50	0.45	0.53	552	96	61.3
c-$AgIn_5S_8$/ZnS	160	160	2.35	0.50	0.49	568	103	59.7