

Supplementary Material

Synthesis of Zn-Cu-In-S/ZnS Core/Shell Quantum Dots with Inhibited Blue-Shift Photoluminescence and Applications for Tumor Targeted Bioimaging

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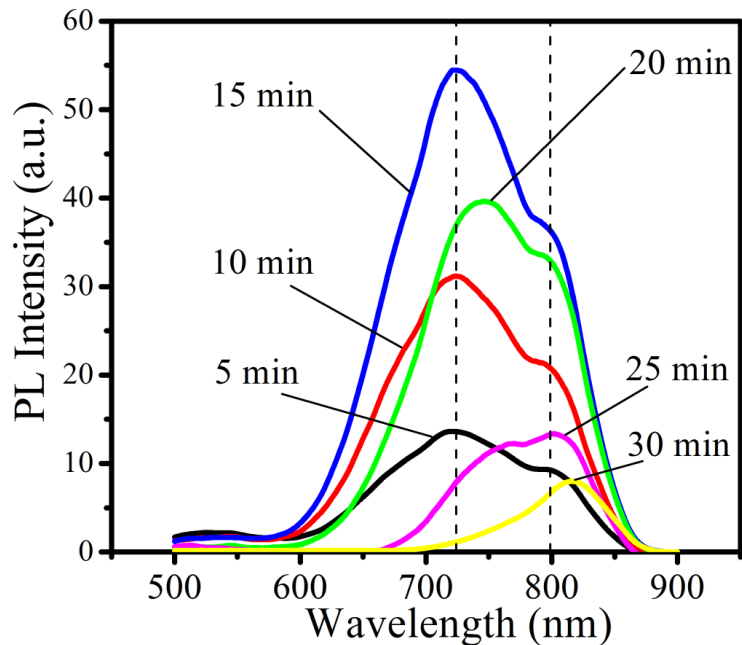


Fig. S1 Temporal evolution of PL emission spectra (b, $\lambda_{\text{ex}} = 470 \text{ nm}$) of CuInS₂ NCs samples in chloroform solution prepared by thermolysis of 0.2 mmol of CuI, 0.2 mmol of In(Ac)₃ and 1 mL of dodecanethiol in 8 mL of ODE at 240 °C for different reaction time.

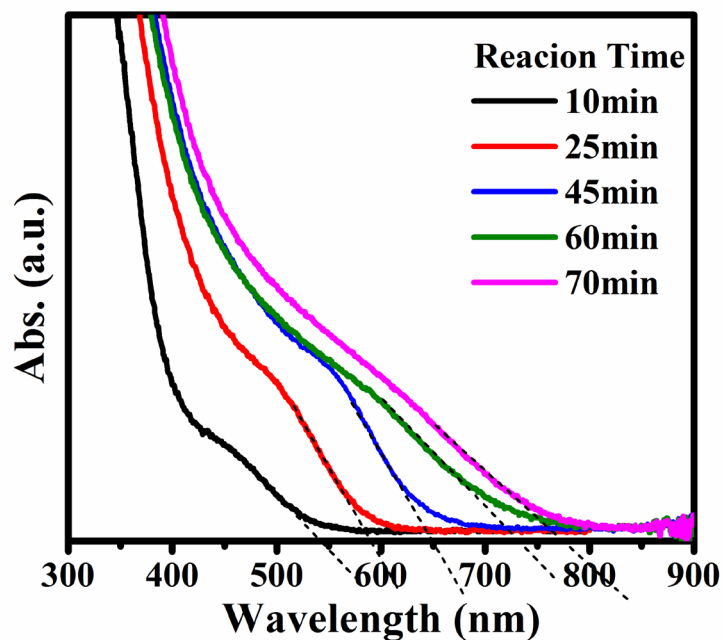


Fig. S2 Determination of the effective bandgaps listed in Table 1. Tangent at the inflection points of the absorption spectra was extrapolated to the Abs=0 axis. Here the effective bandgap was attributed to 2.30 eV, 2.10 eV, 1.91 eV, 1.70 eV and 1.60 eV, which corresponds to wavelength of 542, 590, 650, 730 and 770 nm, respectively.

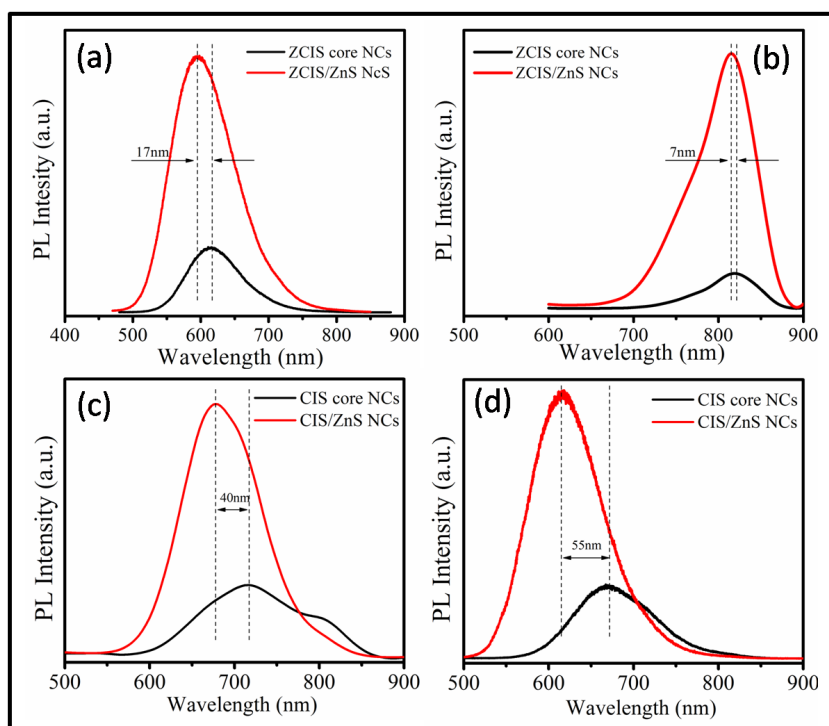


Fig. S3 The PL blue shift properties of the as-prepared ZCIS alloyed NCs (a and b) and CIS core NCs (c and d) synthesized without Zn atom.

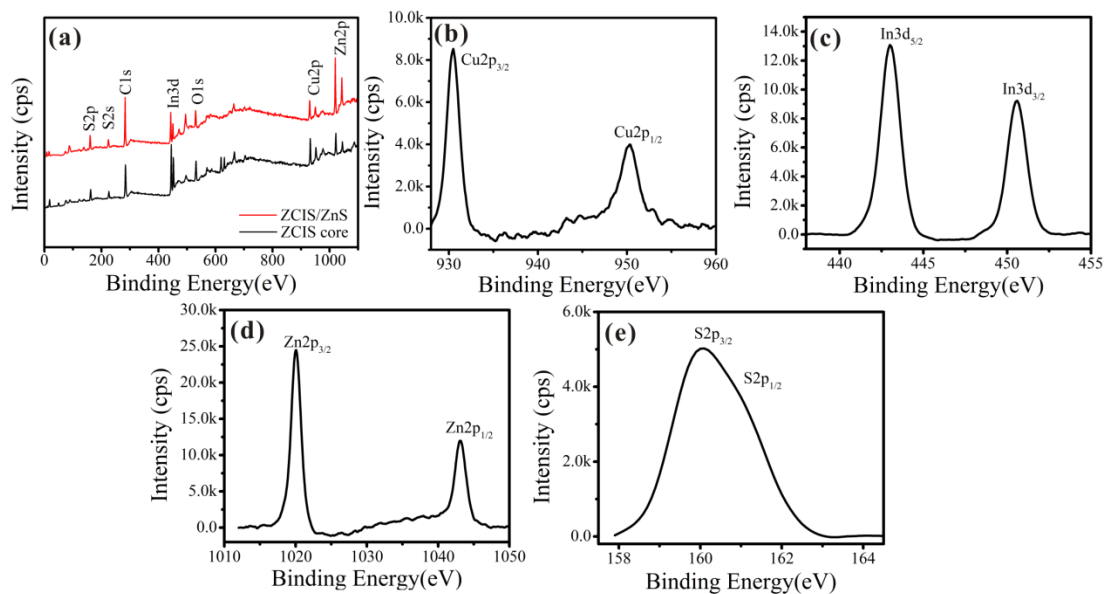


Fig. S4 (a) XPS survey spectrum of ZCIS alloyed NCs and ZCIS/ZnS core/shell NCs, (b) the XPS spectrum of Cu 2p, (c) the XPS spectrum of In 3d, (d) the XPS spectrum of Zn 2p and (e) the XPS spectrum of S 2p of the ZCIS/ZnS NCs.

Table S1. The corresponding quantification reports of XPS.

Sample	Peak	Position BE (eV)	FWHM (eV)	Raw Area (cps)	Mass Conc%	Atomic Conc%
ZCIS NCs	Cu 2p	932.100	1.707	44753.0	20.18	20.34
	In 3d	444.900	1.426	66292.6	43.94	24.52
	Zn 2p	1021.800	1.988	37643.6	16.26	15.93
	S 2p	161.600	2.212	9741.2	19.62	39.21
ZCIS/ZnS	Cu 2p	930.500	1.706	28331.9	13.86	12.22
	In 3d	443.000	1.286	32653.4	23.49	11.46
	Zn 2p	1020.000	1.586	79402.1	37.24	31.91
	S 2p	159.900	2.187	11628.8	25.41	44.41

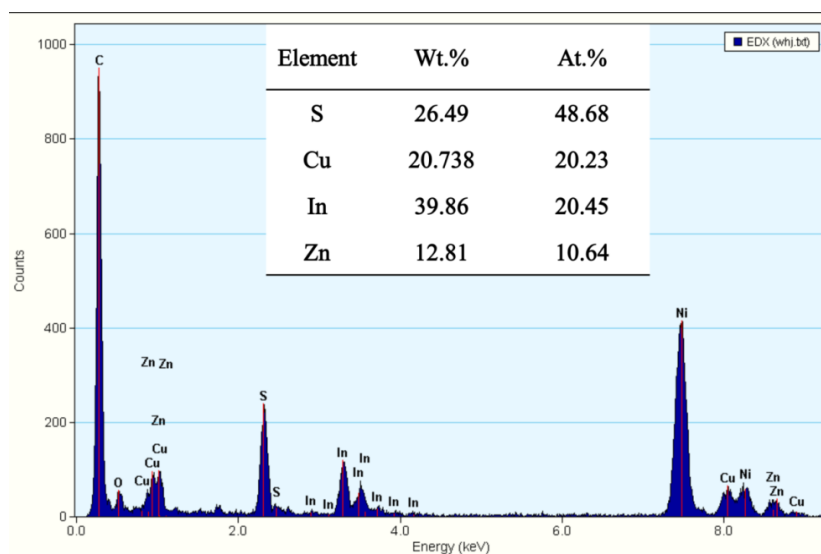


Fig. S5 The energy-dispersive spectroscopy (EDX) of the ZCIS alloyed NCs prepared by thermolysis of 0.2 mmol of CuI, 0.2 mmol of In(Ac)₃, 0.1 mmol of Zn(SA)₂ and 1 mL of dodecanethiol in 8 mL of ODE at 240 °C for 70 min and the quantification analysis

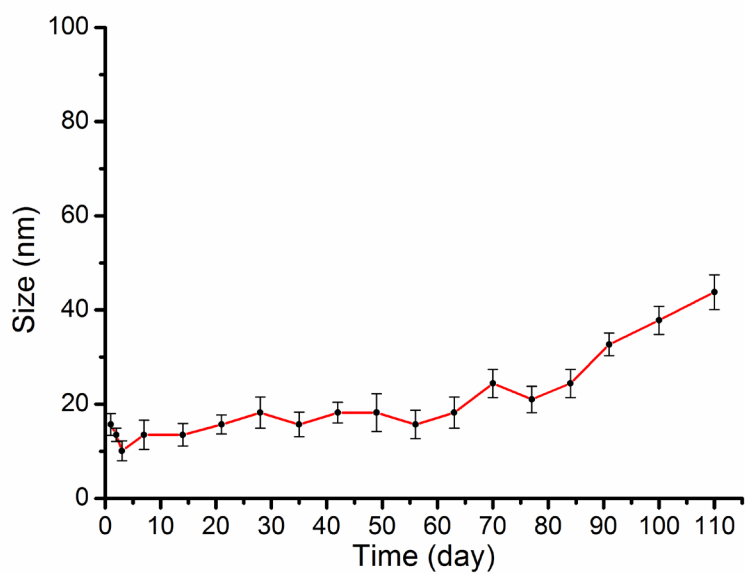


Fig. S6 The recorded hydrodynamic diameter of the water dispersible ZCIS/ZnS QDs in water against time.

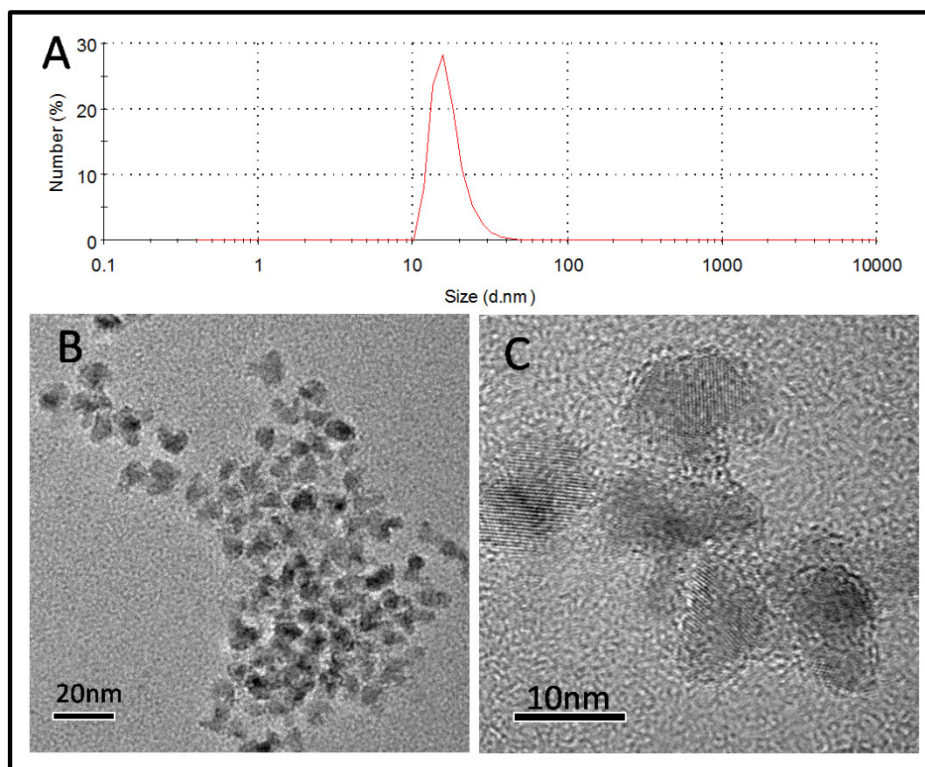


Fig. S7 DLS plot of ZCIS/ZnS QDs in PBS buffer, showing the hydrodynamic diameter (HD) of about 15.7 nm (A); TEM images of the water dispersible ZCIS/ZnS coated with polymer at different magnification (B and C).

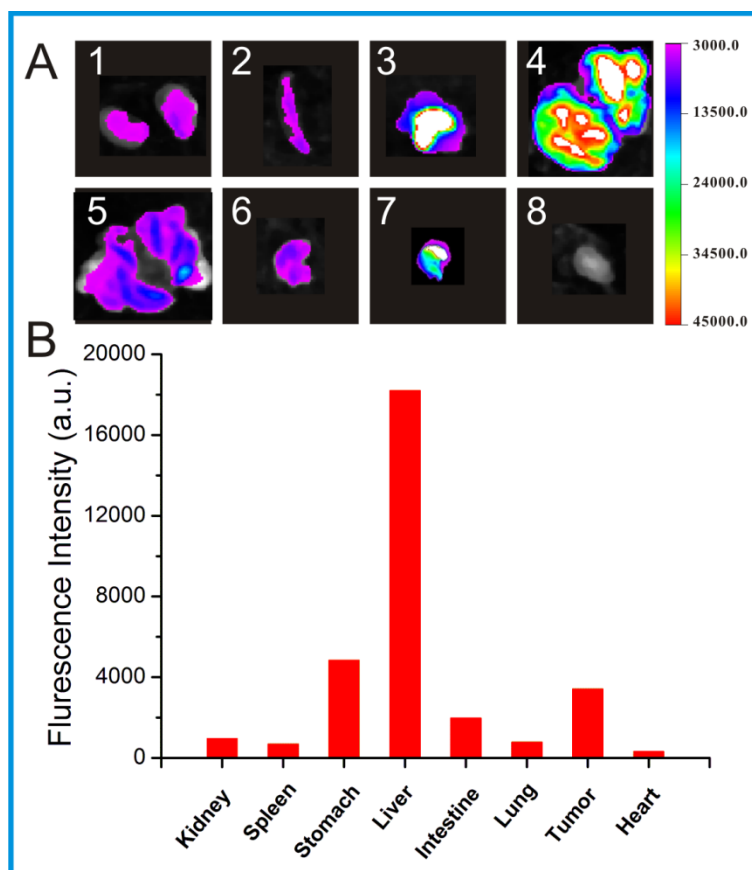


Fig. S8 A. *Ex vivo* NIR fluorescence imaging of the different parts of the mice after dissection at 5 h p.i., In each image 1, kidney; 2, spleen; 3, stomach; 4, liver; 5, intestine; 6, lung; 7, tumor; 8, heart. B. ROI analysis of major organs in *ex vivo* fluorescence imaging after 5 h p.i. of ZCIS/ZnS-cRGD QDs. The data is represented as mean intensity.