Supporting Information

Microwave-assisted synthesis of highly photoluminescent core/shell CuInZnSe/ZnS quantum dots as photovoltaic absorbers

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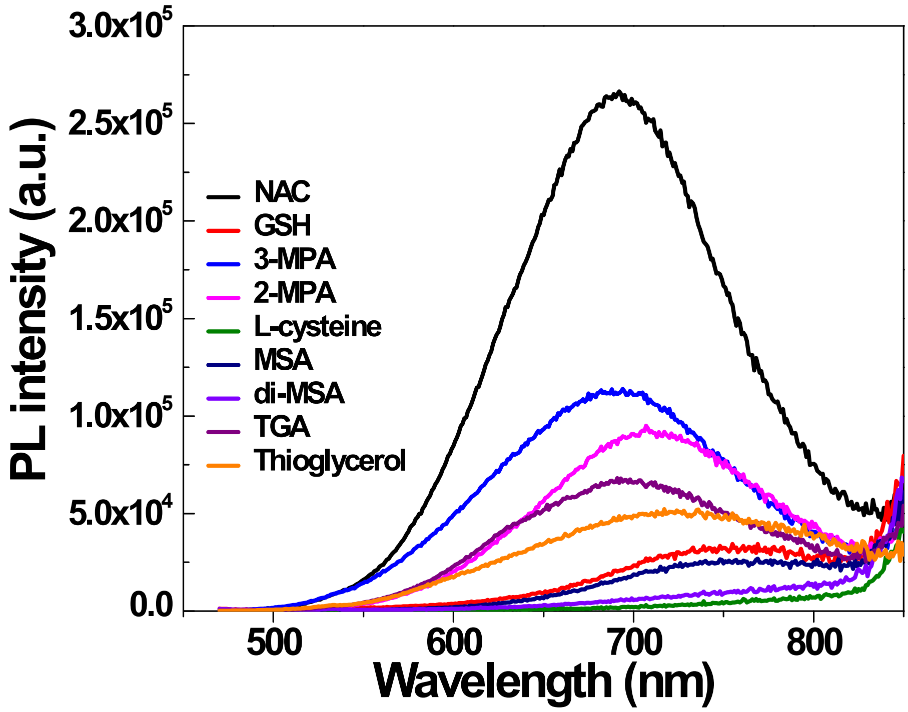

Fig. S1. PL emission spectra of CIZSe/ZnS QDs when varying the capping ligand (NAC : N-acetylcysteine, GSH : glutathione, 3-MPA : 3-mercaptopropionic acid, 2-MPA : 2-mercaptopropionic acid, MSA : mercaptosuccinic acid, di-MSA : dimercaptosuccinic acid, TGA : thioglycolic acid).

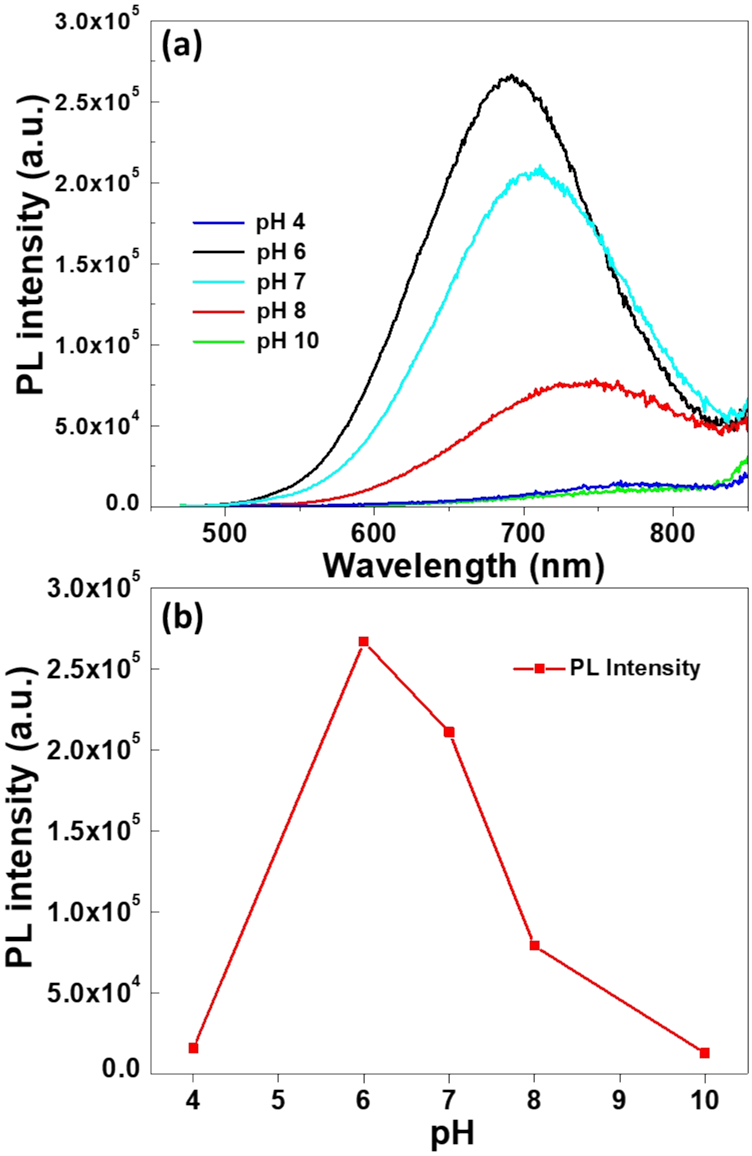

Fig. S2. (a) PL emission spectra of CIZSe/ZnS QDs when varying the pH of the reaction medium (λ_{ex} : 450 nm), (b) PL intensity of CIZSe/ZnS QDs vs pH.

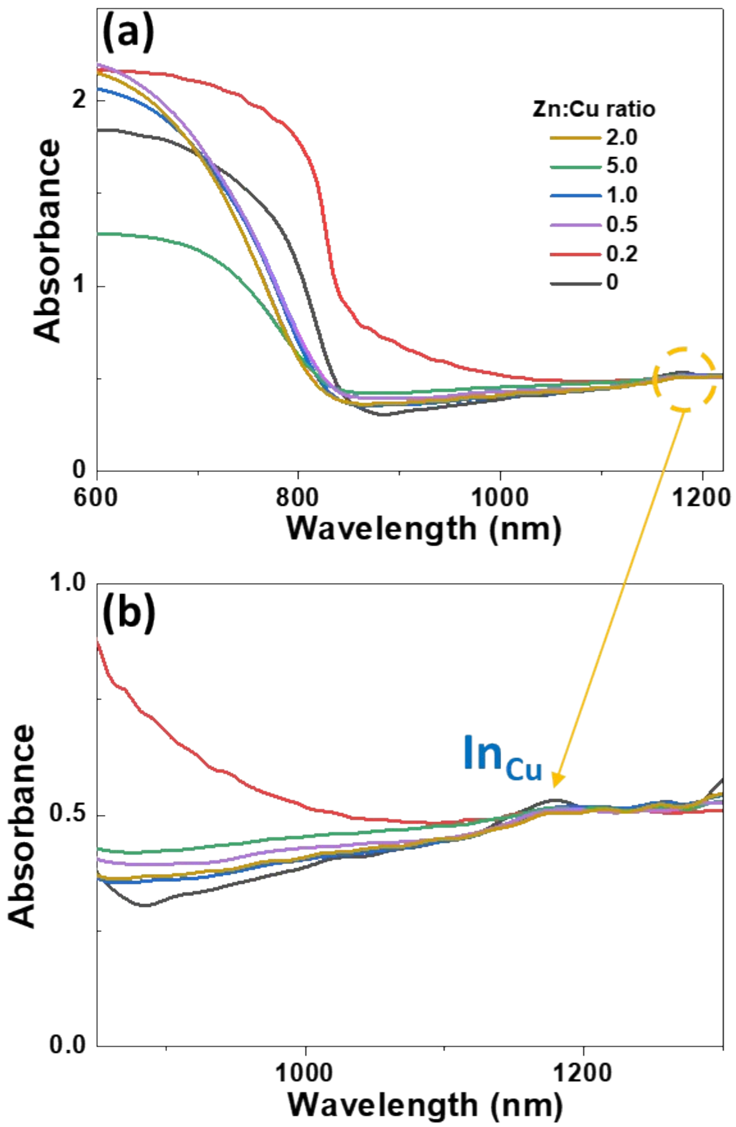

Fig. S3. UV-visible-near infrared diffuse reflectance spectra of CIZSe/ZnS QDs when varying the Zn:Cu ratio.

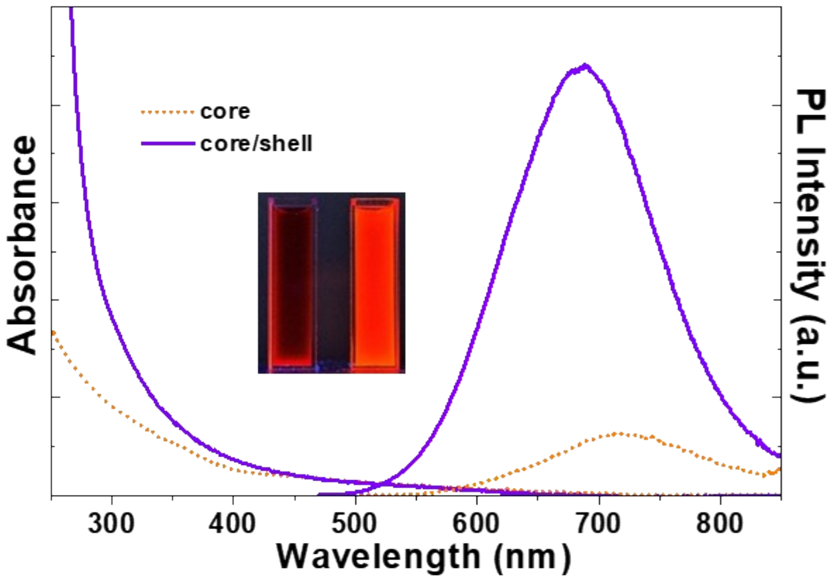

Fig. S4. UV-visible absorption and PL emission spectra of CIZSe (orange dotted lines) and core/shell CIZSe/ZnS QDs (violet lines). The synthesis of the CIZSe core was conducted using a Zn:Cu ratio of 0.5. PL emission spectra were recorded after excitation at 450 nm. The inset is a digital photograph of CIZSe and CIZSe/ZnS QDs colloidal dispersions under UV illumination.

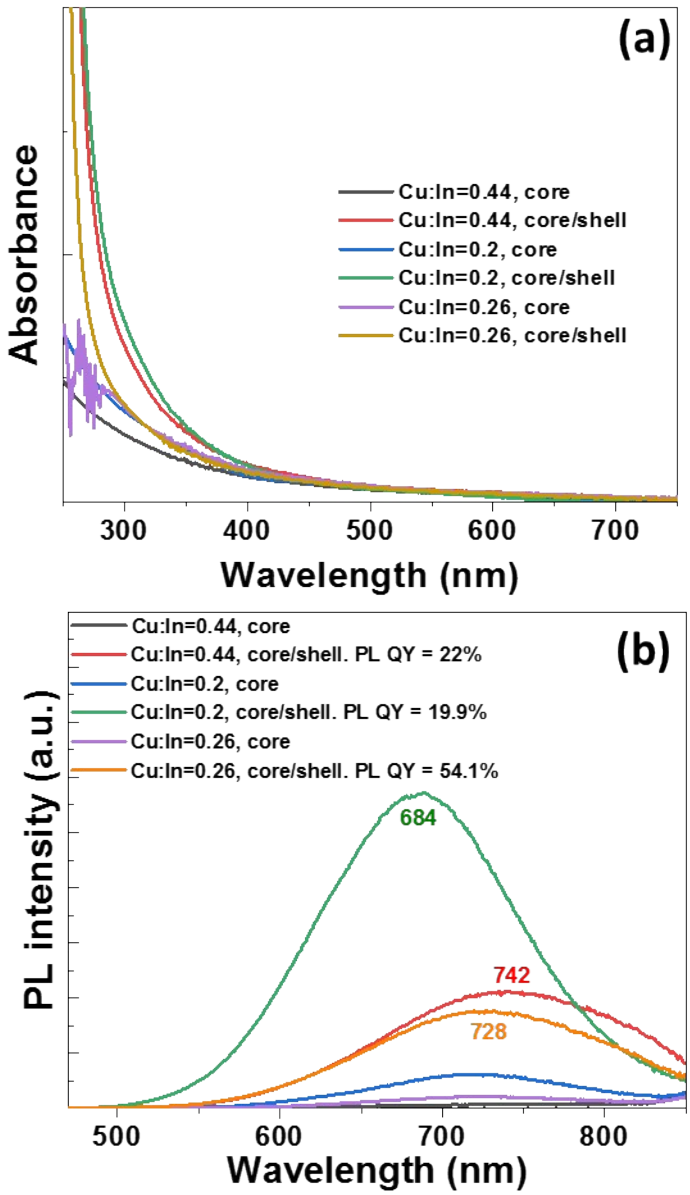

Fig. S5. (a) UV-visible and (b) PL emission spectra of CIZSe and CIZSe/ZnS QDs when varying the Cu:In molar ratio.

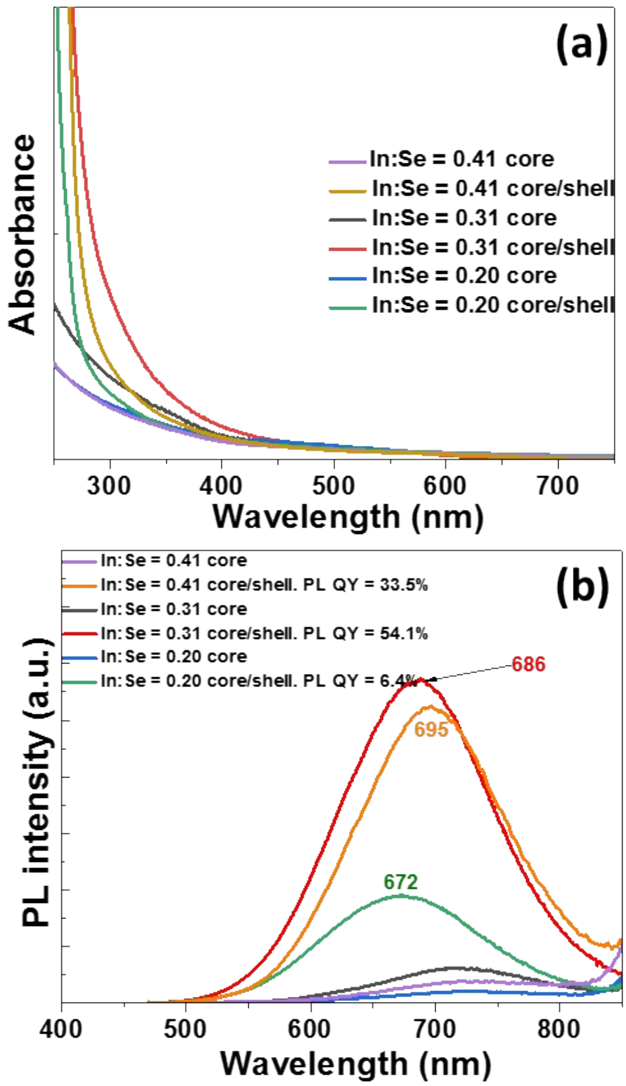

Fig. S6. (a) UV-visible and (b) PL emission spectra of CIZSe and CIZSe/ZnS QDs when varying the In:Se molar ratio.

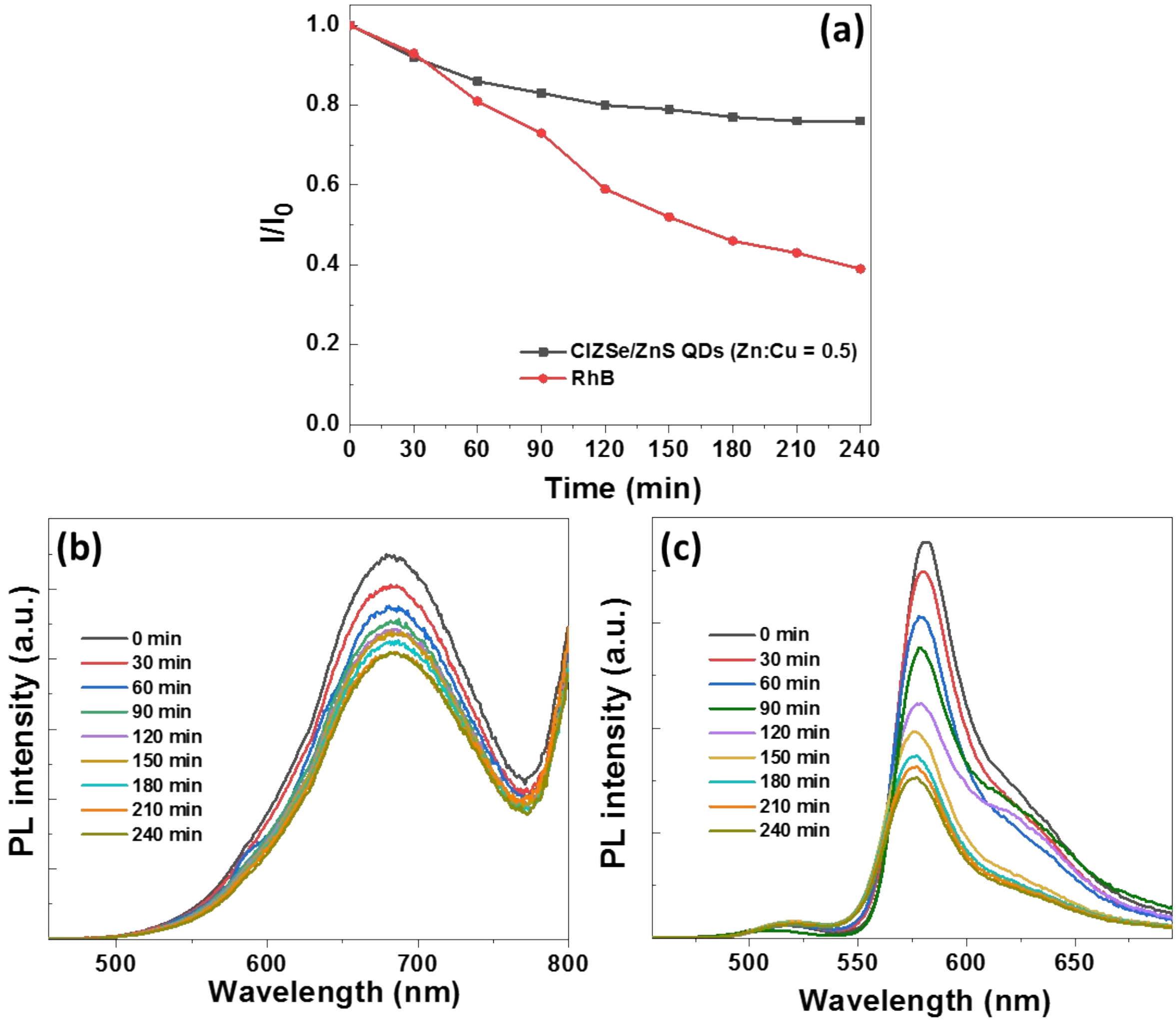

Fig. S7. (a) Photostability of CIZSe/ZnS (Zn:Cu = 0.5) and Rhodamine B under the continuous irradiation of a Hg/Xe lamp (light irradiance of 50 mW/cm^2). Evolution of PL emission spectra of (b) CIZSe/ZnS QDs and (c) Rhodamine B during the irradiation.

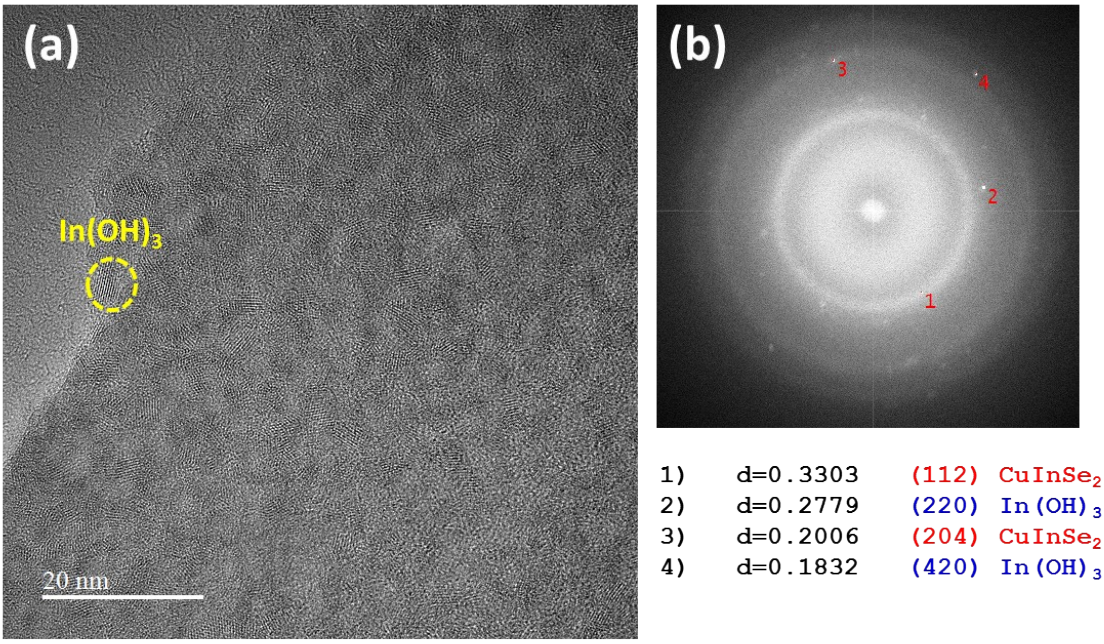

Fig. S8. (a) TEM image of CIZSe/ZnS QDs prepared with a Zn:Cu ratio of 2.0, (b) the associated SAED pattern showing the co-existence of CIZSe/ZnS and $In(OH)_3$ in the sample. The observed diffraction rings correspond to the (112) and (204) planes of the chalcopyrite tetragonal structure of CIZSe/ZnS QDs and to the (220) and (420) planes of cubic $In(OH)_3$.

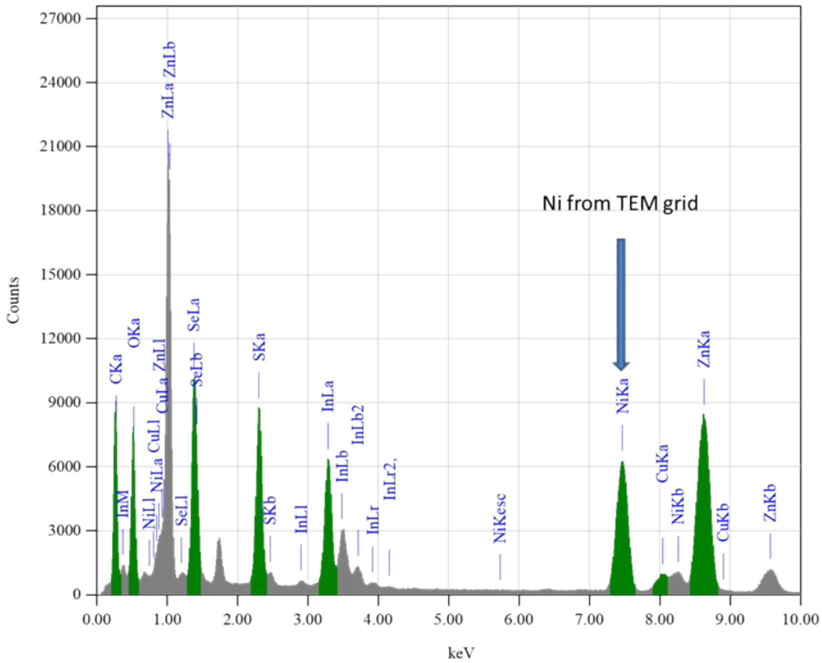

Fig. S9. EDX analysis of CIZSe/ZnS (Zn:Cu = 0.5).

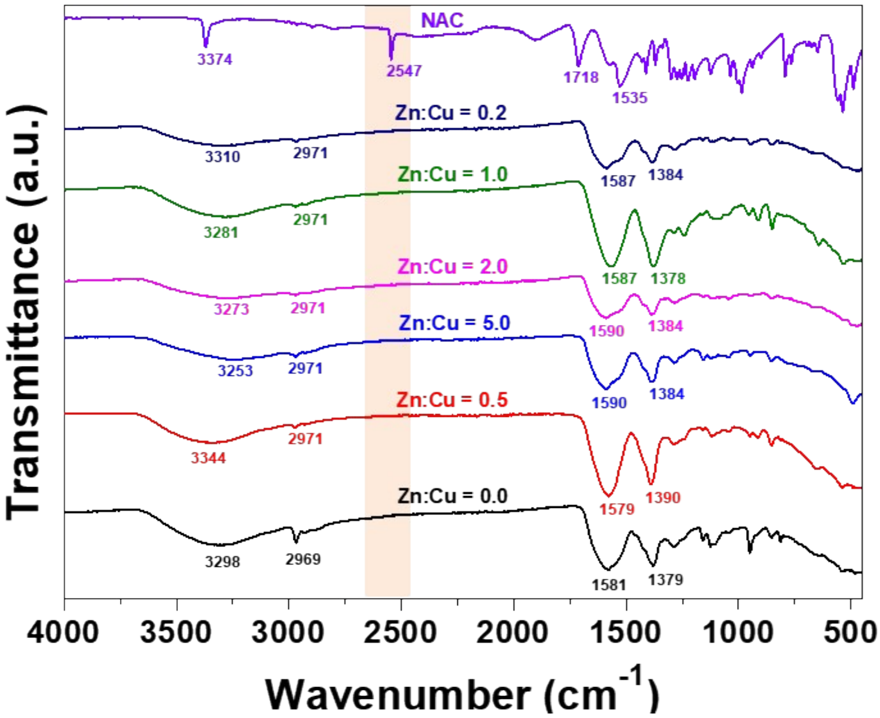

Fig. S10. FT-IR spectra of NAC and CIZSe/ZnS QDs.

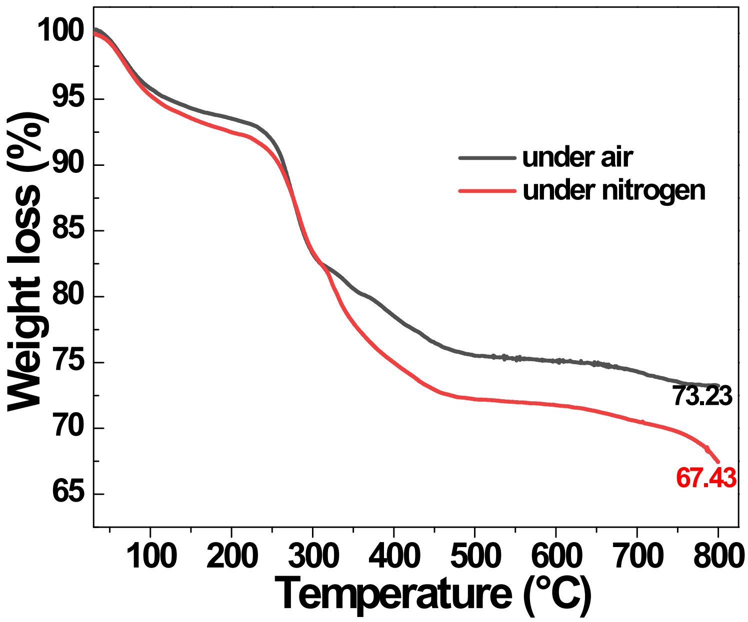

Fig. S11. TGA traces of CIZSe/ZnS QDs under air and under nitrogen.

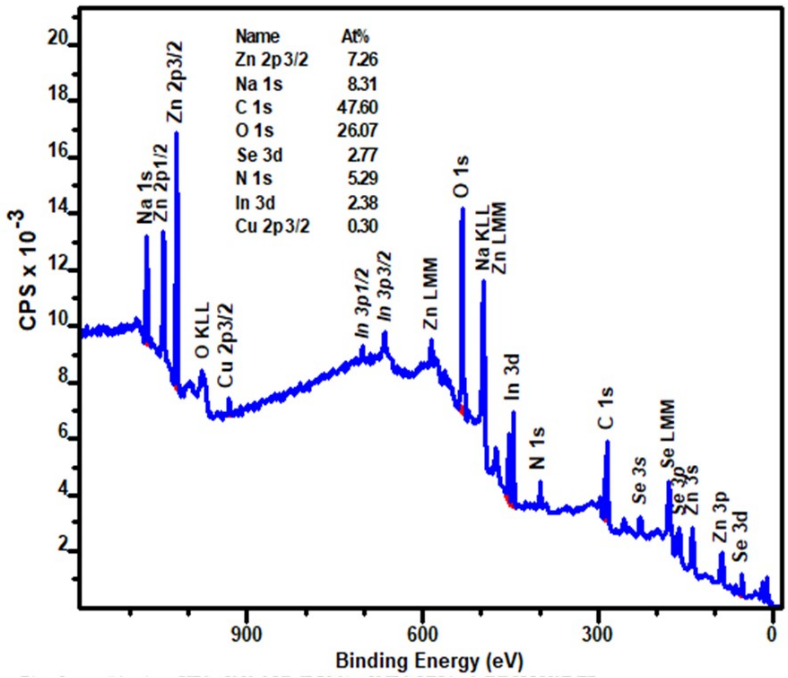

Fig. S12. XPS overview spectrum of CIZSe/ZnS QDs.

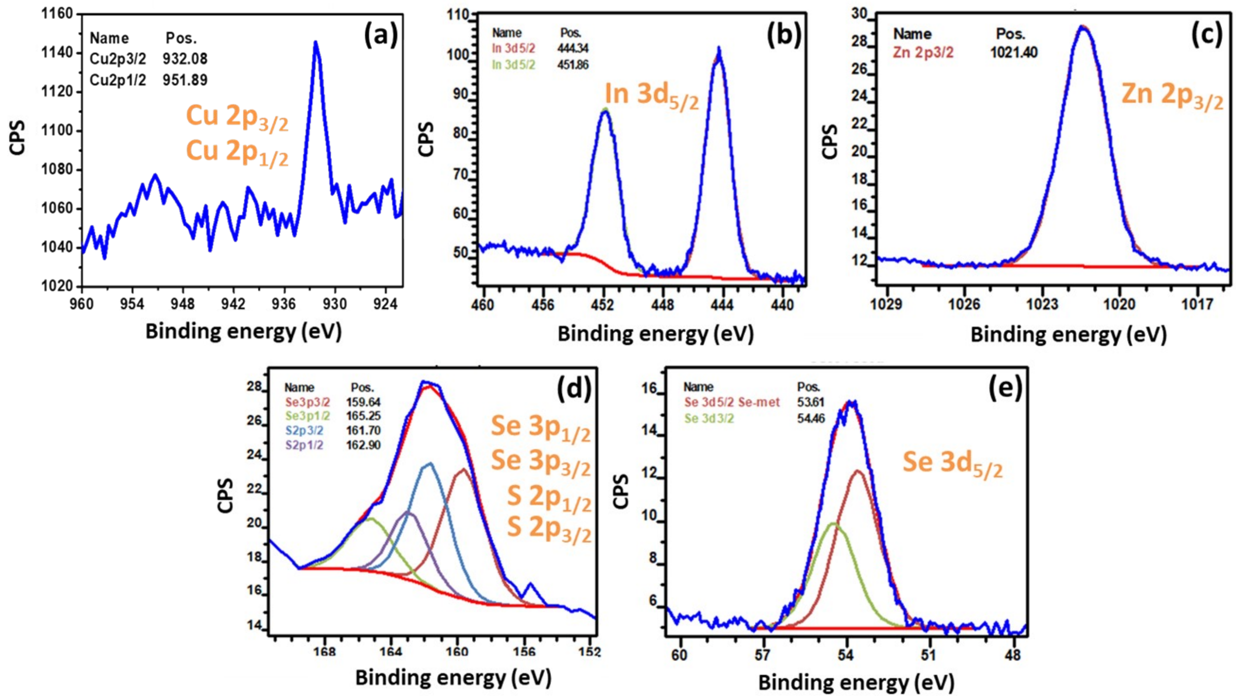

Fig. S13. HR-XPS spectra of (a) Cu 2p, (b) In 3d, (c) Zn 2p, (c) Se 3p and S 2p and (e) Se 3d.

Table S1. Theoretical and experimental Cu/In/Zn molar ratio determined by ICP/OES.

Zn:Cu	**Theoretical Cu/In/Zn molar ratio**	**Cu/In/Zn molar ratio determined by ICP/OES**
0	1/3.3/28	1/2.8/9.3
0.2	1/4/33.8	1/3.1/10.5
0.5	1/10/85	1/7.4/25.2
1	1/6.6/57	1/5.4/18.8
2	1/10/86	1/8.1/25.2
5	1/20/171	1/16.4/61.5

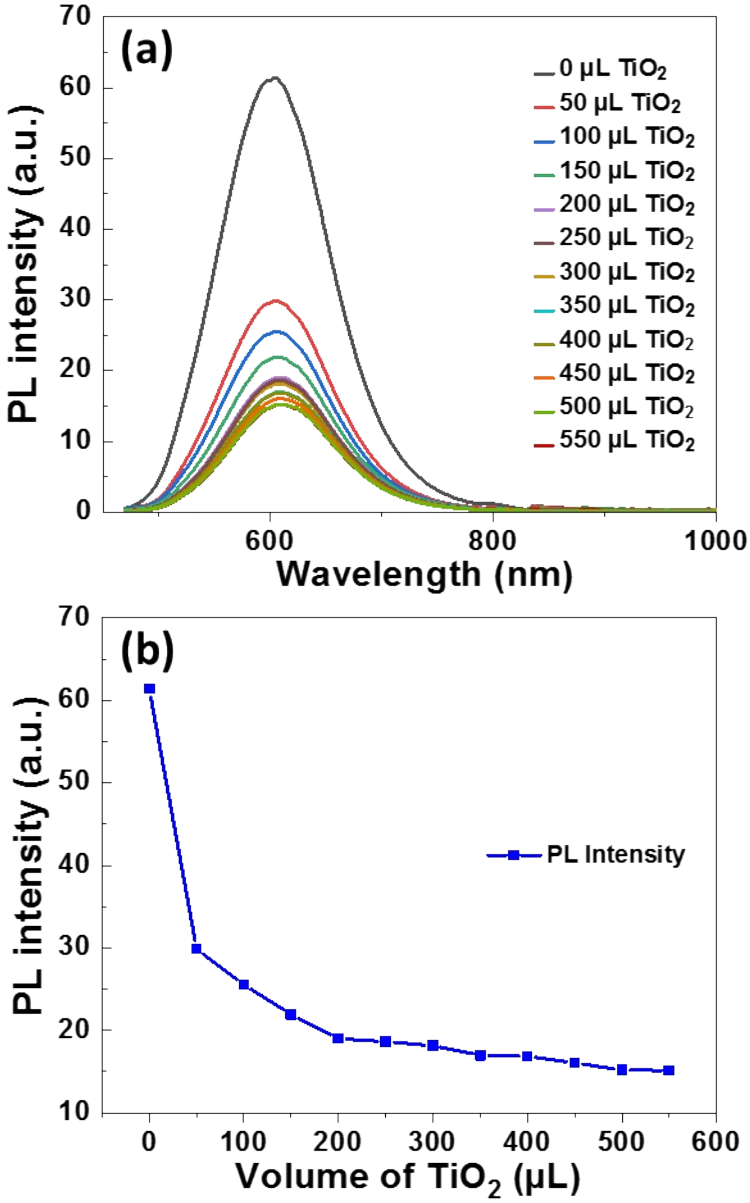

Fig. S14. (a) PL emission spectra of CIZSe/ZnS QDs before and after addition of increasing amounts of a TiO_2 colloid (50 µL of TiO_2 is added in increments to 3 mL of a QDs dispersion in water), (b) PL intensity vs volume of TiO_2 colloid added.