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# Supporting Information

## The facile one-step aqueous synthesis of near-infrared emitting $Cu^+$ doped CdS quantum dots as fluorescence bioimaging probes with high quantum yield and low cytotoxicity

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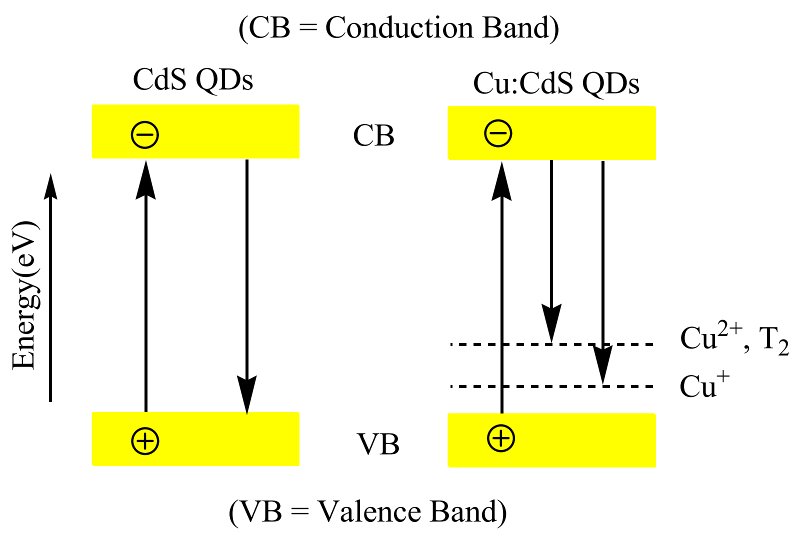

Fig. S1 Scheme of the mechanism for Cu dopant emission.

Table. S1 Previous Cu:CdS QDs properties.

| **Sulfer source** | **Heating atmosphere** | **Solvent** | **Temp. (℃)** | **$Cu^{+}$ or $Cu^{2+}$** | **λmax (nm)** | **QY%** | **Cell imaging** | **Ref.** |
|---|---|---|---|---|---|---|---|---|
| Thiourea | $N_2$ | aqueous | 100 | $Cu^{+}$ | 586 | 21.86 | KB | 1 |
| $Na_2S$ | Air | aqueous | 100 | $Cu^{2+}$ | 722 | <10 | HeLa | 2 |
| Sulfur powder | Air | organic | 220 | $Cu^{+}$ | 680 | 20-30 | - | 4 |
| Dodecanethiol | Air | organic | 200 | $Cu^{+}$ | 707 | 15.8 | - | 7 |
| $H_2S$ gas | Air | organic | 100 | $Cu^{2+}$ | 680 | - | - | 8 |
| Sulfur powder | Air | organic | 220 | $Cu^{2+}$ | 710 | 65 | - | 24 |
| Thiourea | Air | aqueous | 95 | $Cu^{+}$ | 466-612 | 20 | - | 25 |

SI. 1

The photoluminescence quantum yield (PLQY) of as-prepared $Cu^{+}$:CdS QDs was counted by FLS 920 fluorescence spectrophotometer (Edinburgh, Britain) inherent calculator using the formula as:

$QY_{QDs} = \int L_{emission} / \int E_{slovent} - \int E_{sample}$

$L_{emission}$ = Sample emission

$E_{slovent}$ = Solvent excitation

$E_{sample}$ = Sample excitation

The consequence was almost the same with the F-4500 fluorescence spectrophotometer (Hitachi, Japan) which was calculated by manual computation expression as follows:

$$QY_{QDs} = QY_{dye} \times \frac{A_{QDs}}{A_{dye}} \times \left(\frac{n_{QDs}}{n_{dye}}\right)^{2} \times \frac{1-10^{-D_{dye}}}{1-10^{-D_{QDs}}}$$

where A was the integrated area, n was the refractive index, and D was the optical density of QDs and dye. Moreover, the integral method was accurate and simple comparing to the traditional process.

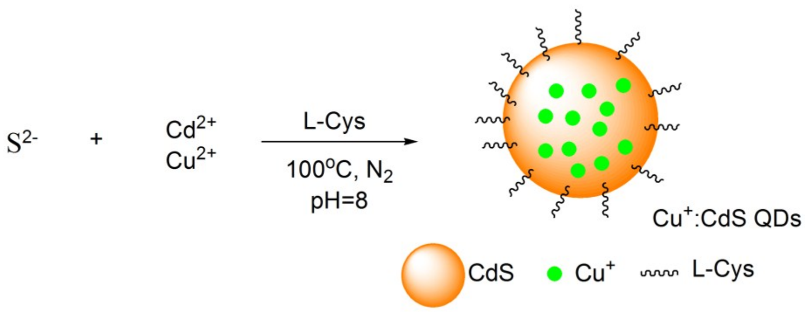


Fig. S2 Synthesis of water soluble $Cu^{+}$ doped CdS quantum dots via one-step method.

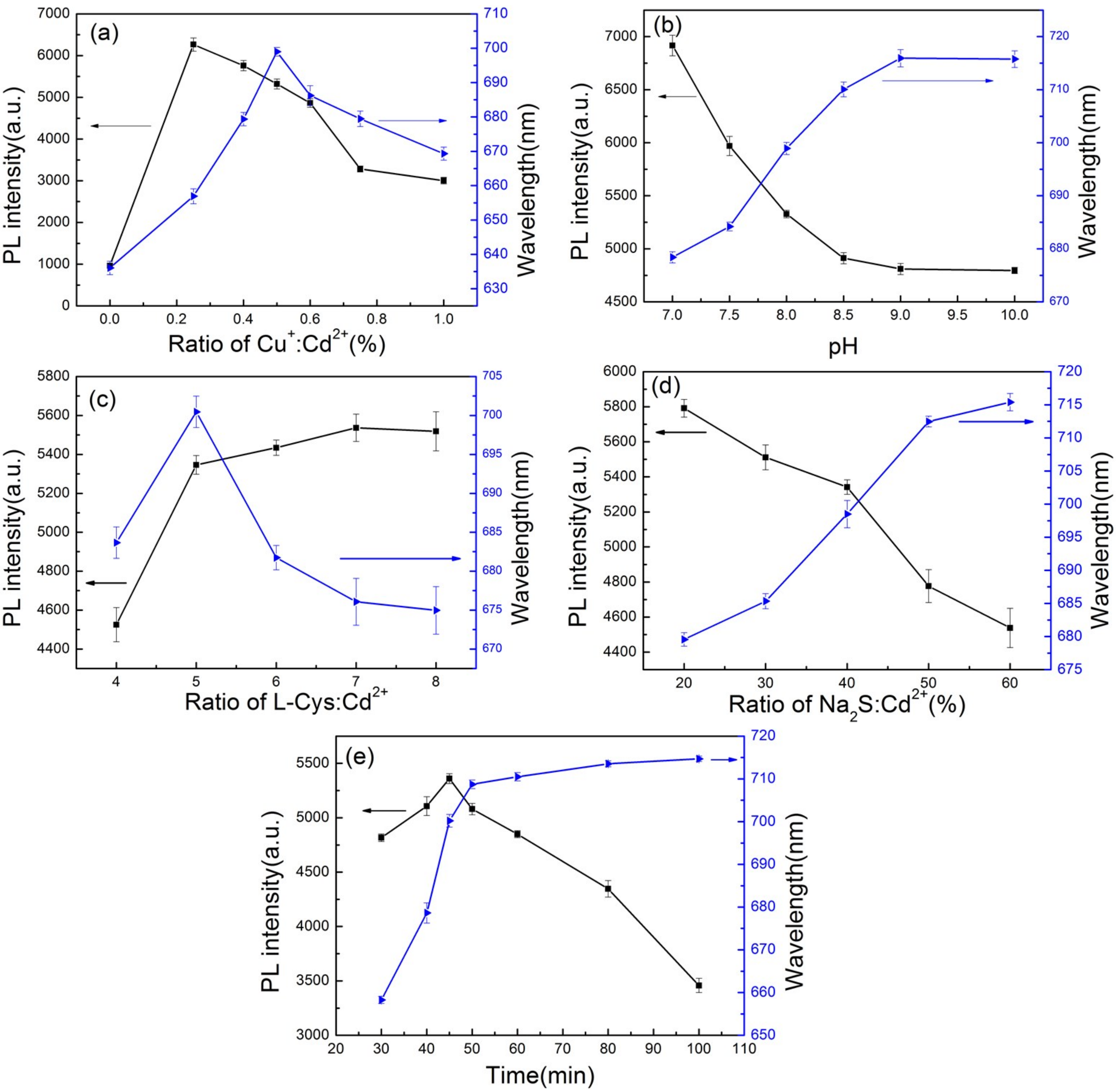


Fig. S3 (a) The emission wavelength and PL intensity of the $Cu^{+}$:CdS QDs synthesized with different Cu dopants amount. (b) Influence of pH on the emission wavelength and PL intensity of the $Cu^{+}$:CdS QDs. (c) The emission wavelength and PL intensity of the $Cu^{+}$:CdS QDs with different concentration of L-Cys. (d) The emission wavelength and PL intensity of the $Cu^{+}$:CdS QDs with different ratios of $Na_2S:Cd^{2+}$. (e) Influence of reflux time on the emission wavelength and PL intensity of the $Cu^{+}$:CdS QDs.

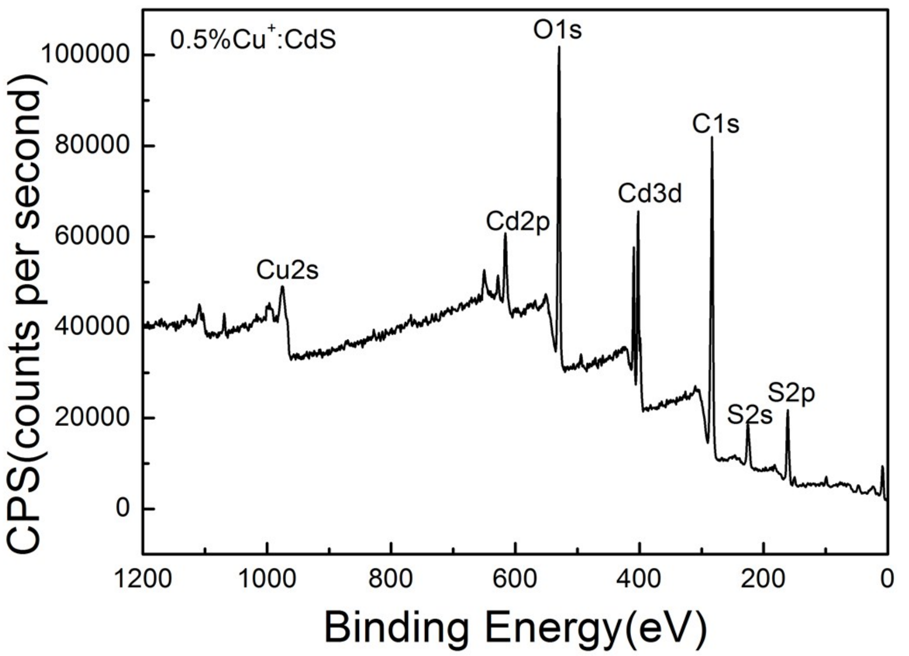


Fig. S4 XPS spectra of the $Cu^+$:CdS QDs.

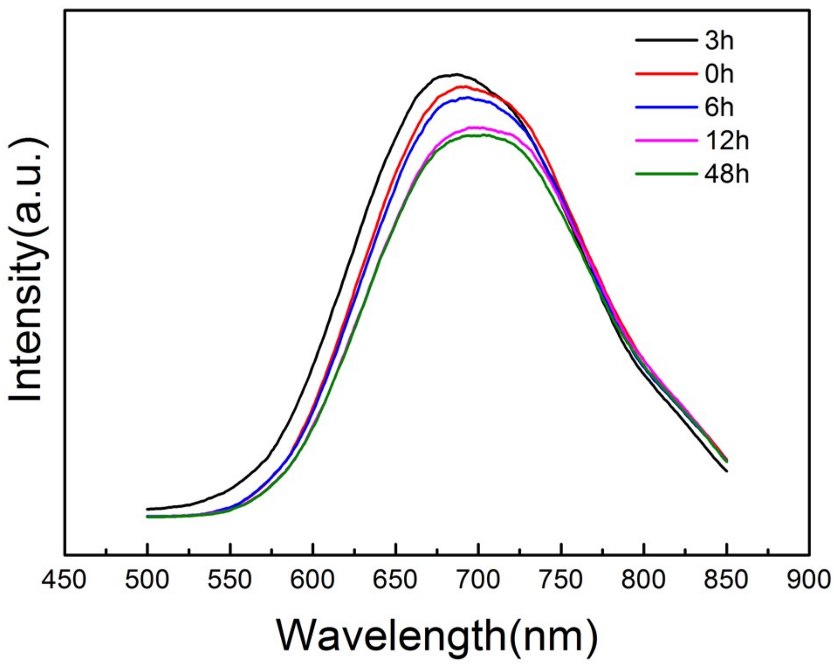


Fig. S5 The PL spectra of the $Cu^+$:CdS QDs synthesized in the optimal conditions in $N_2$ atmosphere after 0, 3, 6, 12, 48 hours.

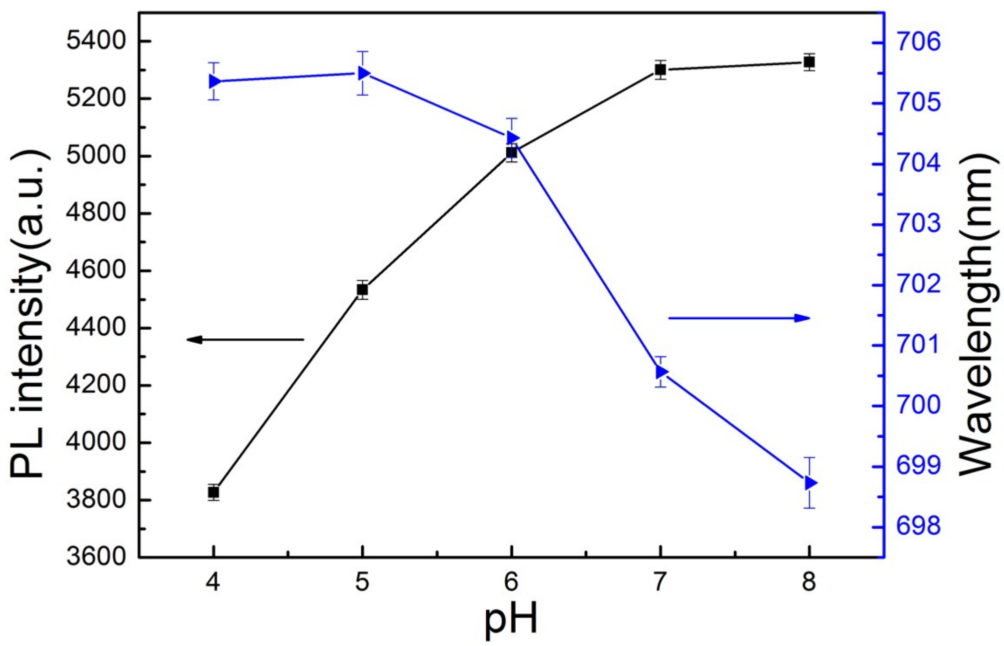


Fig. S6 The effects of pH on the fluorescence properties of the as-prepared $Cu^+$:CdS QDs.

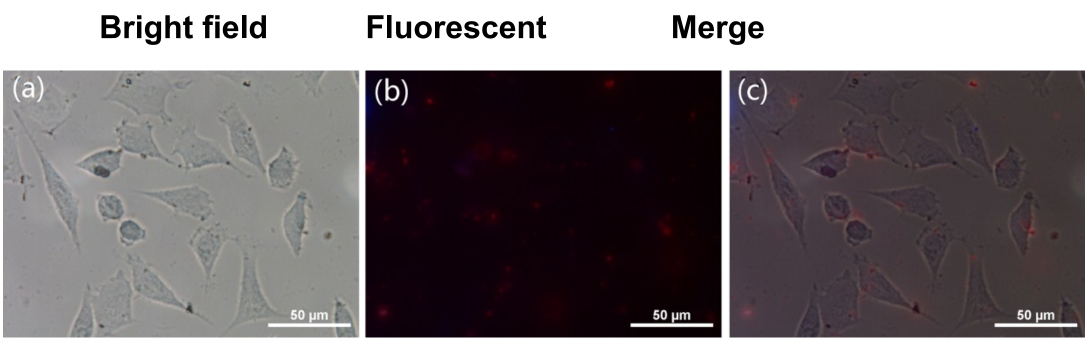

Fig. S7 Fluorescence images of 3T3 cells. (a) Bright field image, (b) fluorescent image and (c) merged image cells incubated for 4 hours with 20 μg/mL Cu:CdS QDs synthesized at optimal conditions in air atmosphere.

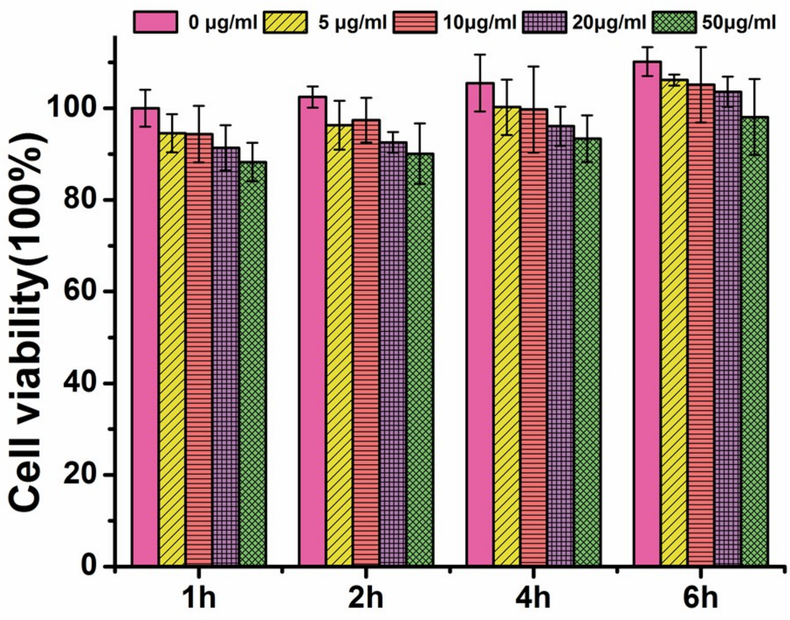


Fig. S8 Effect of the d-dots prepared in air atmosphere on the viability of HeLa cells. The viability of HeLa cells in vitro measured by MTT assay. The HeLa cells were incubated for 1 2, 4, 6 hours with different concentrations (0, 5, 10, 20, 50 μg/mL) of the Cu:CdS QDs prepared in air atmosphere.