

Supplementary information

Calculation of E_g and particle size

The optical band gaps of CIS QDs (Direct-gap semiconductor) could be roughly estimated by empirical formula.³⁷

$$(\alpha hv)^2 = A(hv - E_g) \dots\dots ①$$

Where A is a constant that depends on the transition probability, E_g is the optical band gap energy, h is the Plank constant and ν is the frequency. The E_g of the CIS QDs was calculated by extrapolating a straight line to the $(\alpha hv)^2 = 0$ axis in the plots of the $(\alpha hv)^2$ versus optical band gap energy. In this way, the optical band gaps of CIS QDs were determined. It is worthy note that the first absorption peak intensity in UV-vis spectrum should below 1.0 so as to reduce the experiment error. Assuming that the transition probability was 1, the equation could be simplified as listed below.

$$(\alpha hv)^2 = hv - E_g \dots\dots ②$$

Known function

$$hv = h \frac{C}{\lambda} = \frac{1240}{\lambda} \dots\dots ③$$

The equation could be translated into the equation 4 listed below.

$$\left(\alpha \frac{1240}{\lambda}\right)^2 = \frac{1240}{\lambda} - E_g \dots\dots ④$$

In the equation 4, α is the absorption value in the UV-vis spectrum that could be detected by UV-vis spectrophotometer, while λ is the detection wavelength. For example, figure 1S (a) shows the UV-vis spectrum of CIS QDs sampling at 25min prepared at 230°C. According to the equation 4, figure 1S (b) was achieved by treating $(\alpha hv)^2$ as Y axis and hv as X axis. The $E_g(2.790\text{eV})$ could

be estimated by extrapolating a straight line to the $(\alpha h\nu)^2 = 0$ axis in the plots of the $(\alpha h\nu)^2$ versus optical band gap energy.

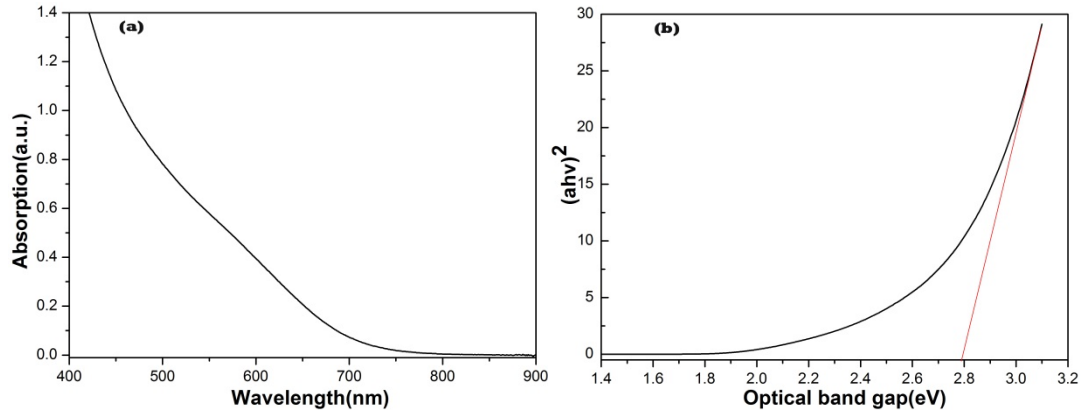


Figure 1. (a) The UV-vis spectrum of CIS QDs sampling at 25min prepared at 230°C. (b) $(\alpha h\nu)^2$ versus optical band gap obtained on the basis of equation 4.

According to the calculation results of optical band gaps, the particle size of CIS QDs could be obtained by modified effective mass approximation equation.³⁸⁻³⁹

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2R^2} \left(\frac{1}{m_e^*} + \frac{1}{m_h^*} \right) - \frac{1.786e^2}{4\pi\epsilon R} \dots\dots \textcircled{2}$$

Where ΔE_g is the shift of band gap of the CIS QDs with respect to the bulk semiconductor, R is the particle radius, \hbar is the reduced Planck's constant, m_e^* (1.46×10^{-31} Kg) is effective electron mass, and m_h^* (1.18×10^{-30} Kg) is the effective hole mass, ϵ (9.74×10^{-11} F/m) are the vacuum permittivity and dielectric constant of the bulk material, respectively. Hence, the radius of CIS could be theoretically calculated by corresponding UV-vis absorption spectra.