Electronic Supplementary Information

One-pot solution synthesis of shape-controlled copper selenide nanostructures and their potential applications in photocatalysis and photothermal therapy

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Experimental Details:

Calculation method for the photothermal conversion efficiency[1]

According to Roper's report, the total energy balance between input and dissipation for the system can be given as:

$$\sum_i m_i C_i \frac{dT}{dt} = Q_{NC} + Q_{sys} - Q_{out} \tag{1}$$

Where *m* and C are the mass and heat capacity of water, respectively, T is the solution temperature, Q_{NC} is the energy absorbed by NCs, Q_{sys} is the energy imputed by the pure water system, and Q_{out} is heat dissipation of the system.

The heat absorbed (Q_{NC}) by PEGylated Cu_2Te NCs can be shown as:

$$Q_{NC} = I(1 - 10^{-A_{808}})\eta \tag{2}$$

Where *I* is incident laser power in W, η is the photothermal conversion efficiency, and A_{808} indicates the absorbance of the PEGylated Cu_2Te NCs at 808 nm.

Q_{out} is linear with system temperature, as expressed as:

$$Q_{out} = hS(T - T_{surr}) \tag{3}$$

Where *h* is heat transfer coefficient, *S* is the surface area of the container, and T_{surr}

is ambient temperature of the surroundings.

When the system reaches a steady state temperature (T_{max}), the heat input and output are balanced:

$$Q_{NC} + Q_{sys} = Q_{out} = hS(T_{\max} - T_{surr}) \tag{4}$$

After the laser is removed, the Q_{NC} + Q_{sys} = 0, reducing the Eq. (1)

$$\sum_i m_i C_i \frac{dT}{dt} = -Q_{out} = -hS(T - T_{surr}) \tag{5}$$

Rearranging the Eq. (5) would give

$$dt = -\frac{\sum_i m_i C_i}{hS} \frac{dT}{(T - T_{surr})} \tag{6}$$

And integrating, give the expression

$$t = -\frac{\sum_i m_i C_i}{hS} \ln \frac{T - T_{surr}}{(T_{\max} - T_{surr})} \tag{7}$$

A system time constant τ_s is defined as:

$$\tau_s = -\frac{\sum_i m_i C_i}{hS} \tag{8}$$

And θ is introduced using the maximum system temperature, T_{max}

$$\theta = \frac{T - T_{surr}}{(T_{\max} - T_{surr})} \tag{9}$$

Substituting Eq. (8) and (9) giving:

$$t = -\tau_s \ln \theta \tag{10}$$

Therefore, the time constant for heat transfer from the system τ_s can be determined by applying the linear time data from the cooling period vs. negative natural logarithm of driving force temperature (θ)

Since Q_{sys} can be obtained directly as

$$Q_{sys} = hS(T_{\max,H_2O} - T_{surr}) \tag{11}$$

Eq. (4) can be given as:

$$Q_{NC} = I(1 - 10^{-A_{808}})\eta = hS(T_{\max} - T_{\max,H_2O}) \tag{12}$$

Also

$$hS = -\frac{\sum_i m_i C_i}{\tau_s} \quad (13)$$

References

1. D. K. Roper, W. Ahn and M. Hoepfner, *J Phys Chem C Nanomater Interfaces*, 2007, **111**, 3636-3641.

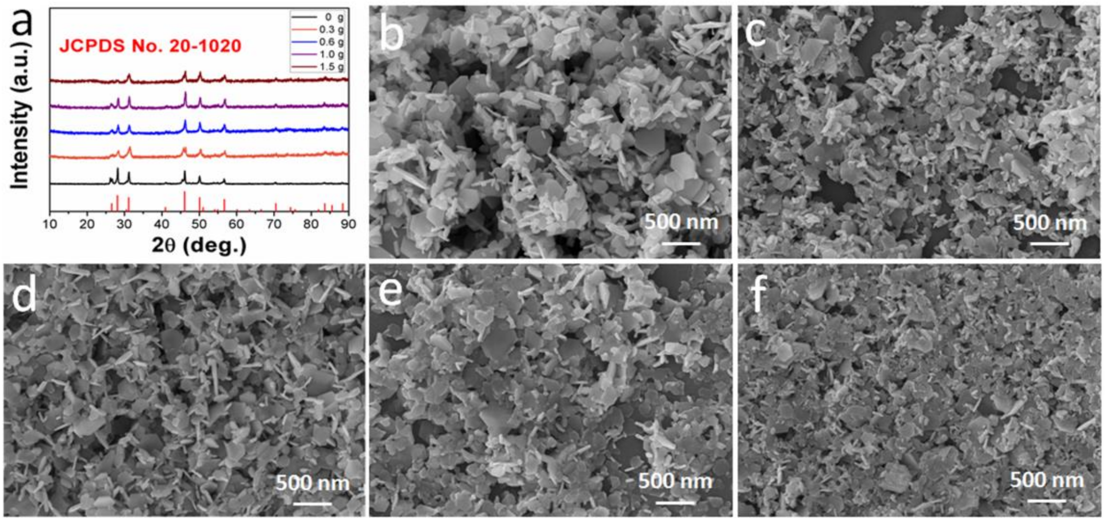

Fig. S1 Characterization of CuSe nanoplates obtained from reactions with different amount of PVP. a) XRD characterization of obtained CuSe nanoplates; SEM images of CuSe nanoplates by using different amount of PVP: b) 0 g; c) 0.3 g; d) 0.6 g; e) 1.0 g and f) 1.5 g.

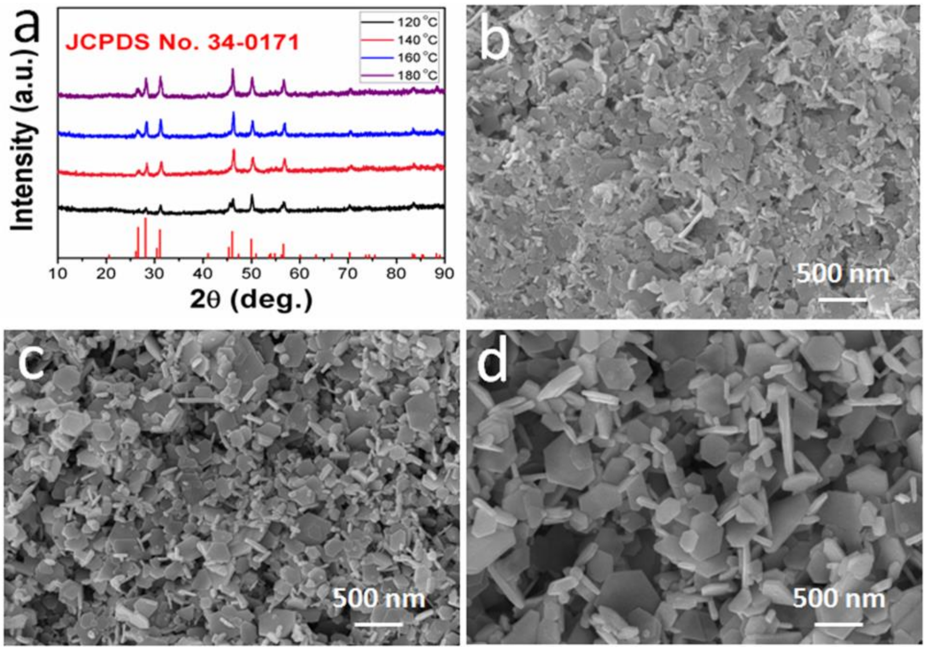

Fig. S2 Characterization of CuSe nanoplates obtained from reactions with different reaction temperatures. a) XRD characterization of obtained CuSe nanoplates; SEM images of CuSe nanoplates with different reaction temperatures: b) 120 °C; c) 140 °C and d) 180 °C.

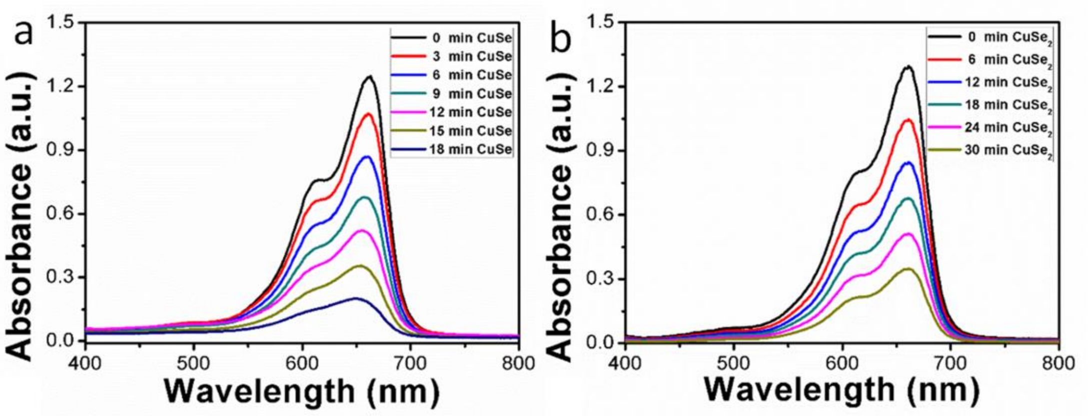

Fig. S3 UV-vis absorption spectra of MB aqueous solution in the presence of a) CuSe nanoplates and b) $CuSe_2$ nanosheets with H_2O_2 (1.0 mL) during photodegradation.

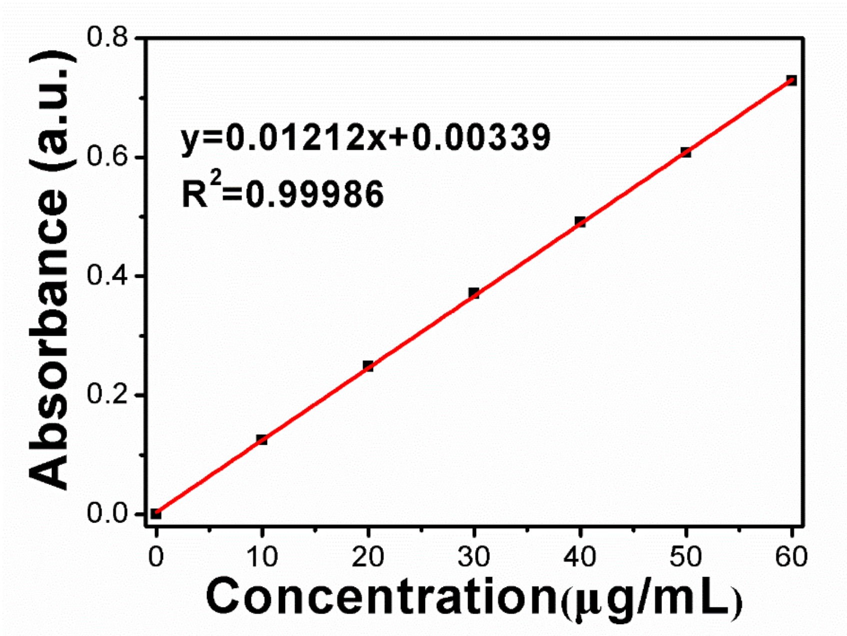

Fig. S4 The absorbance of CuSe nanoplates at 808 nm increased as the concentration of CuSe nanoplates increased.

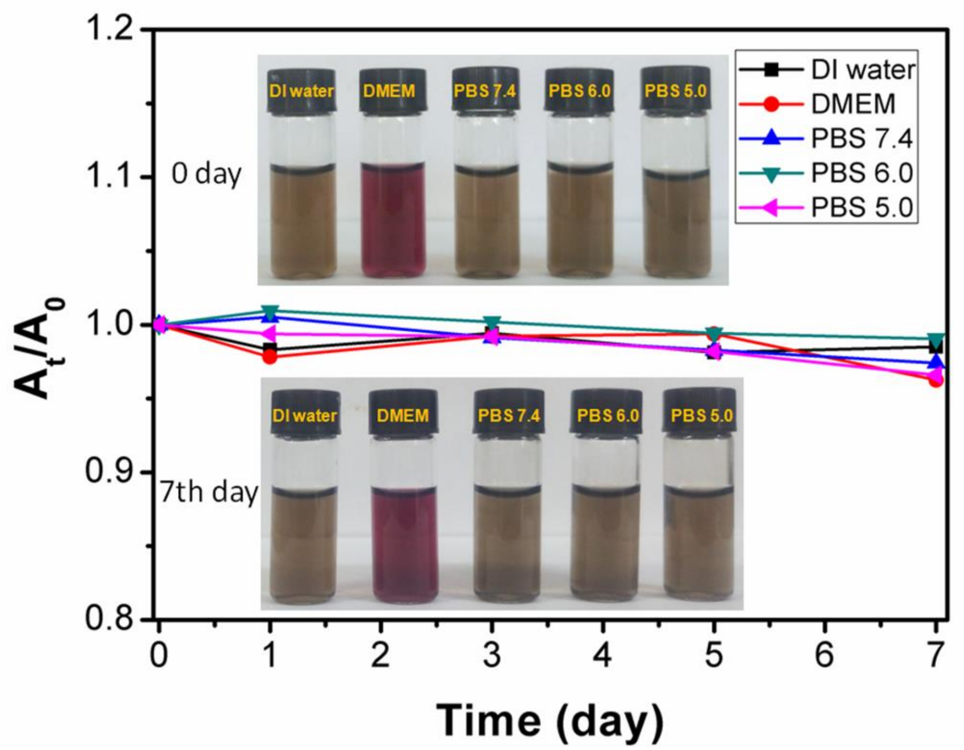

Fig. S5 The stability of CuSe nanoplates characterized in different medium, including DI water, DMEM cell culture medium, PBS with different pH (7.4, 6.0 and 5.0); insets: photographs of CuSe nanoplates dispersions.