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Electronic Supplementary Information

$CuS@mSiO_2$-PEG core-shell nanoparticles as a NIR light responsive drug delivery nanoplatform for efficient chemo-photothermal therapy

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Calculation of the photothermal conversion efficiency

The photothermal conversion efficiency of $CuS@mSiO_2$-PEG core-shell nanoparticles was measured according to the references[1-3]. The aqueous solution of the $CuS@mSiO_2$-PEG core-shell nanoparticles (100 ppm) underwent continuous irradiation of 980 nm laser (0.72 W/cm^2) until steady state temperature was reached. Then the laser was shut off, and the aqueous solution was naturally cooled to environment temperature. The temperature change of the aqueous solution was recorded (Fig. S6a). The η value was calculated as follows:

$$\eta = \frac{hS(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1-10^{-A_{980}})} \qquad (1)$$

Where h is the heat transfer coefficient, S is the surface area of the container, and the value of hS is obtained from the Eq.4 and Figure S6b. The maximum steady temperature ($T_{\max}$) was 33.8 ^{o}C and environmental temperature (T_{Surr}) was 16.0 ^{o}C. The laser power I used in irradiation was 0.277 W. The absorbance of the $CuS@mSiO_2$-PEG core-shell nanoparticles at 980 nm A_{980} was 0.747. Q_{Dis} is heat dissipated from the light absorbed by the solvent and container.

A dimensionless parameter θ is calculated as followed:

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \qquad (2)$$

A sample system time constant τ_s can be calculated as Eq.3.

$$t = -\tau_s \ln(\theta) \qquad (3)$$

According to figure 3b, τ_s was determined and calculated to be 233.80 s.

$$hs = \frac{m_D C_D}{\tau_s} \quad (4)$$

In addition, m_D is 0.3 g and C_D is 4.2 J/g·°C. Thus, according to Eq. 4, *hS* is calculated to be 5.39 mW/ °C.

Q_{Dis} is heat dissipated from the light absorbed by the container itself, and it was determined independently to be 28.97 mW using a container containing pure water.

Thus, substituting according values of each parameters to Eq. 1, the 980 nm laser photothermal conversion efficiency (η) of the CuS@mSiO$_2$-PEG core-shell nanoparticles can be calculated to be 29.5%.

Supplementary Figures

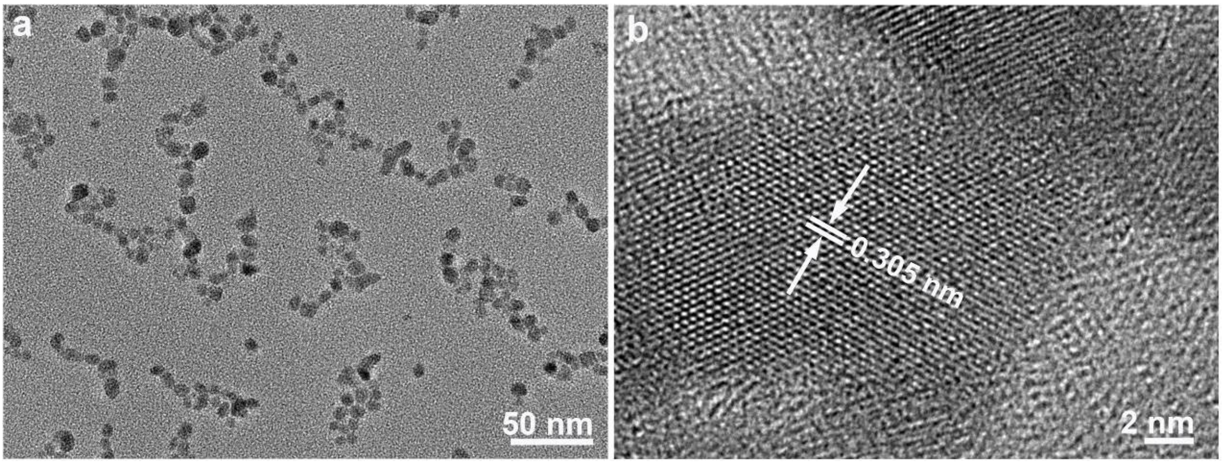

Fig. S1 (a) The TEM image and (b) HRTEM image of CuS nanocrystals

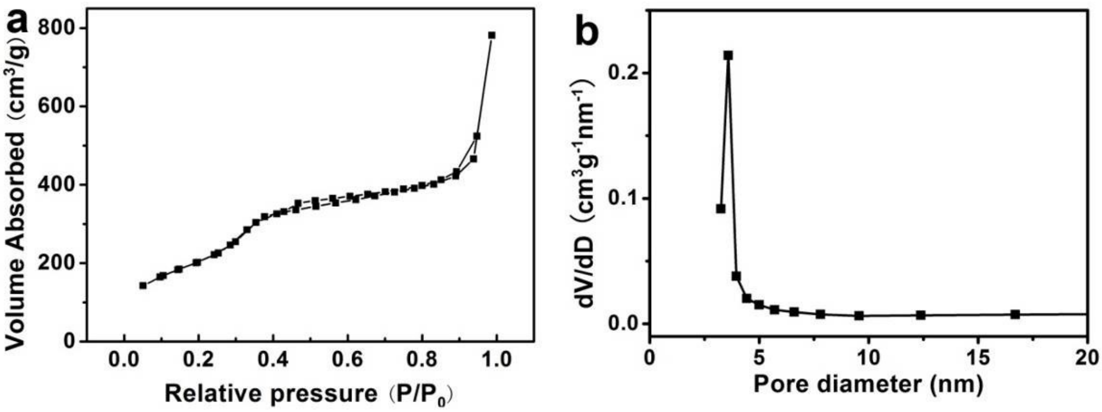

Fig. S2 (a) N_2 adsorption-desorption isotherms and (b) the pore diameter distribution of CuS@mSiO$_2$-PEG core-shell nanoparticles

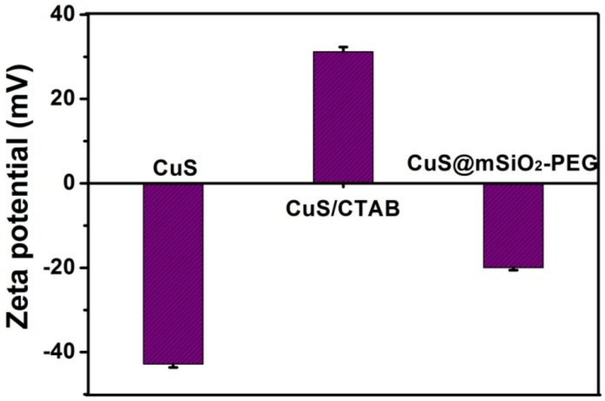

Fig. S3 The Zeta potentials of CuS nanocrystals, CuS/CTAB and CuS@mSiO$_2$-PEG nanoparticles

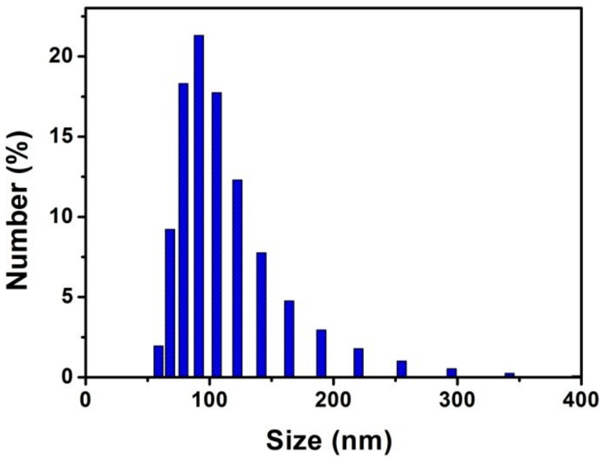

Fig. S4 The size distribution of the CuS@mSiO$_2$-PEG core-shell nanoparticles in the water determined by dynamic light scattering.

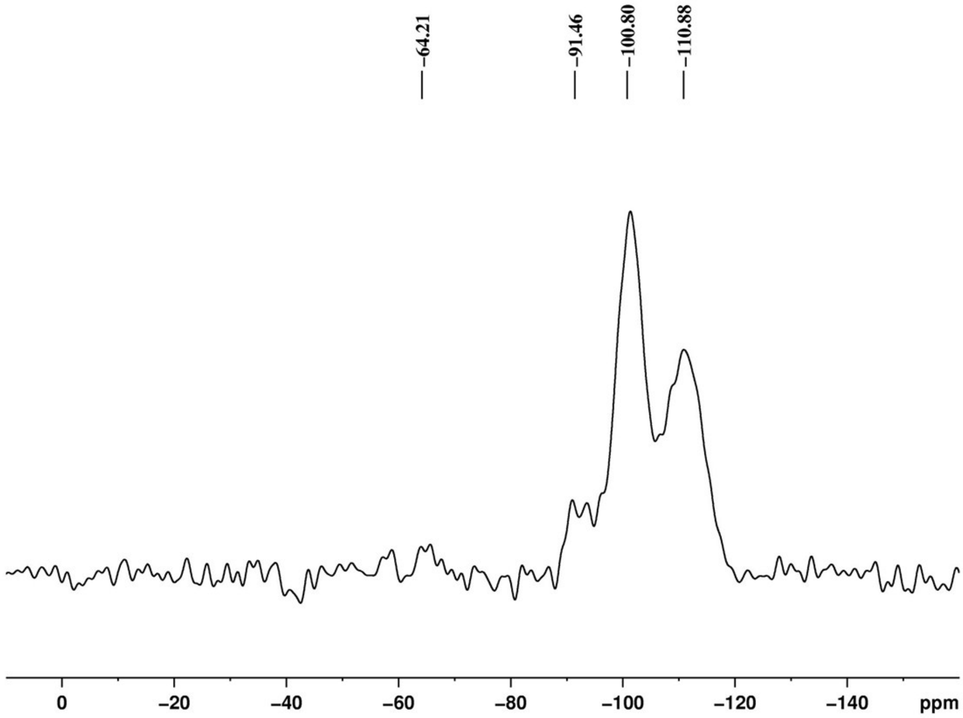

Fig. S5 ^{29}Si NMR spectrum of CuS@mSiO$_2$-PEG nanoparticles

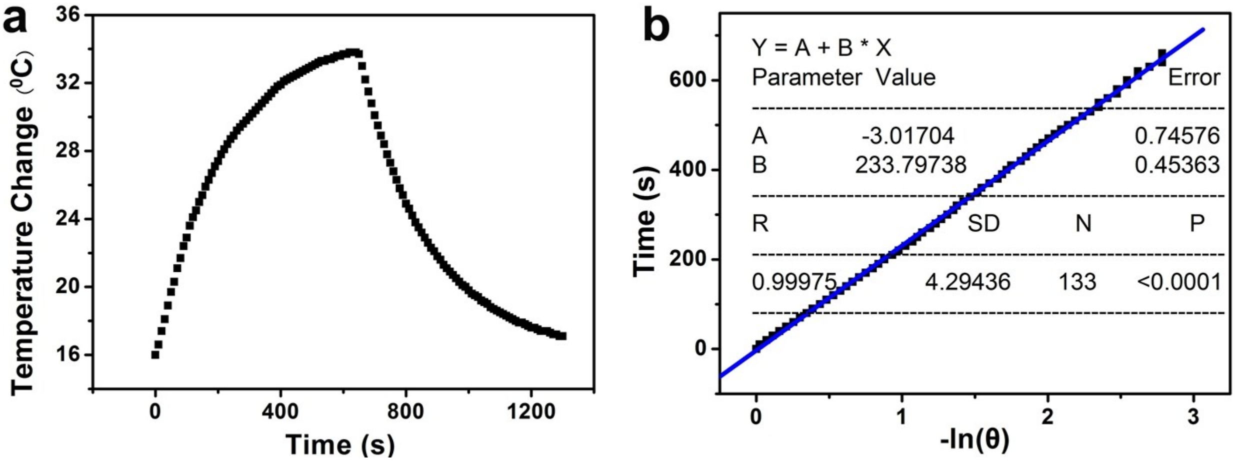

Fig. S6 (a) Photothermal effect of the irradiation of the aqueous solution of the CuS@mSiO$_2$-PEG core-shell nanoparticles (100 ppm) with the NIR laser (980 nm, 0.72 W/cm^2), in which the irradiation lasted for 650 s, and then the laser was shut off. (b) Linear time data versus -ln(θ) obtained from the cooling period of Fig. S6a.

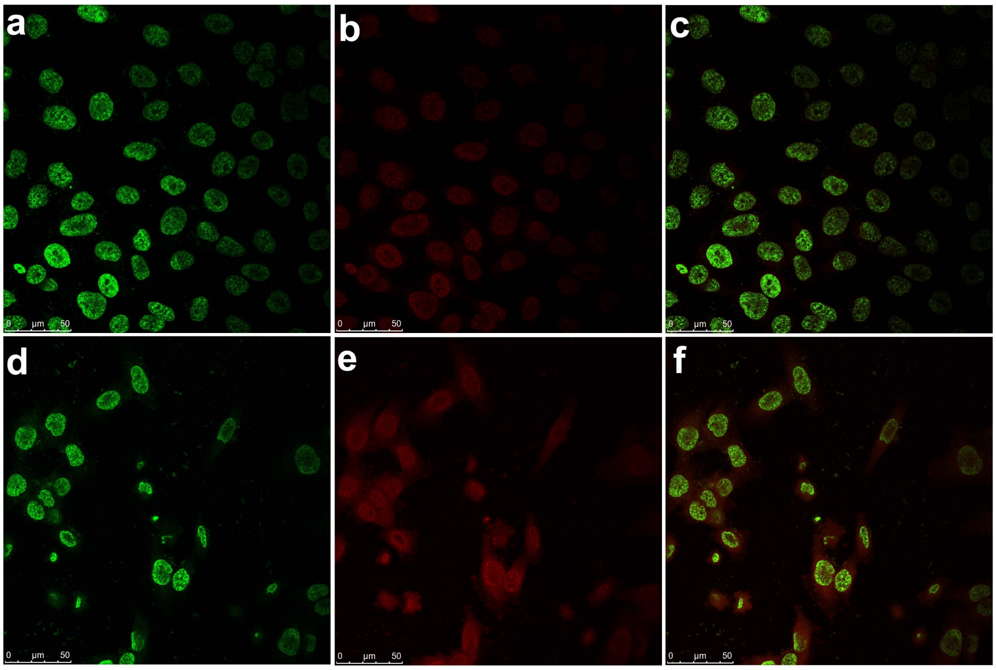

Fig. S7 CLSM images of HeLa cells incubated with CuS@mSiO_2-PEG/DOX for (a-c) 4 h and (d-f) 8 h. For each series, images from left to right can be classified to the nuclei of cells (green, being dyed by Hoechst 33324), DOX fluorescence in cells (red), and the merged images of both above, respectively.

Reference:

1. C. M. Hessel, V. P. Pattani, M. Rasch, M. G. Panthani, B. Koo, J. W. Tunnell and B. A. Korgel, *Nano Lett.*, 2011, **11**, 2560-2566.
2. Q. Tian, F. Jiang, R. Zou, Q. Liu, Z. Chen, M. Zhu, S. Yang, J. Wang, J. Wang and J. Hu, *Acs Nano*, 2011, **5**, 9761-9771.
3. X. Liu, B. Li, F. Fu, K. Xu, R. Zou, Q. Wang, B. Zhang, Z. Chen and J. Hu, *Dalton Trans.*, 2014, **43**, 11709-11715.