Facile Synthesis of Biocompatible Cysteine-coated CuS Nanoparticles with High Photothermal Conversion Efficiency for Cancer Therapy

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Calculation of the photothermal conversion efficiency

The photothermal conversion efficiency of the Cys-CuS NPs was determined according to the previous method. Detailed calculation was given as following:

\[
\eta = \frac{hS(T_{max} - T_{Surr}) - Q_{dis}}{I(1 - 10^{-4\omega})}
\]  \hspace{1cm} (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 3b. The maximum steady temperature \( (T_{max}) \) of the solution of the Cys-CuS NPs was 40.1 °C and environmental temperature \( (T_{Surr}) \) was 18.6 °C. So, the temperature change \( (T_{max} - T_{Surr}) \) of the solution of the Cys-CuS NPs was 21.5 °C. The laser power \( I \) is 0.288 W. The absorbance of the Cys-CuS NPs at 980 nm \( A_{980} \) is 1.187. \( Q_{dis} \) expresses heat dissipated from the light absorbed by the solvent and container.

In order to gain \( hS \), a dimensionless parameter \( \theta \) is introduced as followed:

\[
\theta = \frac{T - T_{Surr}}{T_{max} - T_{Surr}}
\]  \hspace{1cm} (2)

A sample system time constant \( \tau_s \) can be calculated as Eq.3.

\[
t = -\tau_s \ln(\theta)
\]  \hspace{1cm} (3)
According to figure 3b, $\tau_s$ was determined and calculated to be 203.20s.

$$hS = \frac{mD\cdot C\cdot s}{\tau_s} \quad (4)$$

In addition, $m$ is 0.3 g and $C$ is 4.2 J/g·°C. Thus, according to Eq. 4, $hS$ is deduced to be 6.20 mW/ °C.

$Q_{Dis}$ expresses heat dissipated from the light absorbed by the quartz sample cell itself, and it was measured independently to be 31.04 mW using a quartz cuvette cell containing pure water.

Thus, substituting according values of each parameters to Eq. 1, the 980 nm laser heat conversion efficiency ($\eta$) of the Cys-CuS NPs can be calculated to be 38.0%.

The $\tau_s$ of the gold nanorods was determined and calculated to be 218.80 s, $hS$ is deduced to be 5.76 mW/ °C. The absorbance of the gold nanorods at 980 nm $A_{980}$ is 1.062, then the 980 nm laser heat conversion efficiency ($\eta$) of the gold nanorods can be calculated to be 21.3%.

**Supplementary Experimental Section**

Gold nanorods were synthesized by previously described method.\textsuperscript{1,2}

**Supplementary Figures**

![Histogram showing size distribution of Cys-CuS NPs](image)

**Fig.S1** Histogram showing size distribution of Cys-CuS NPs
Fig. S2 The size distribution of the clusters of Cys-CuS NPs determined by dynamic light scattering.
**Fig. S3** TEM images and UV-vis-NIR absorbance spectra of the aqueous solutions of the Cys-CuS NPs with a different mean size: (a) and (b) ~ 18 nm, (c) and (d) ~ 35 nm, (e) and (f) ~ 55 nm.

**Fig. S4** The digital photo (a) and schematic diagram (b) showing the equipment in measuring photothermal performance.

**Fig. S5** (a) TEM images of the synthesized Au nanorods. (b) Absorption spectrum of the aqueous dispersion of the Au nanorods (50 ppm) (c) Photothermal effect of the irradiation of the aqueous solution of the Au nanorods (50 ppm) with the NIR laser (980 nm).
nm, 0.72 W/cm²), in which the irradiation lasted for 660 s, and then the laser was shut off.

(d) Linear time data versus -ln(θ) obtained from the cooling period of Fig. S2c.

![Graph](image)

**Fig. S6** Body weights of mice after PBS and Cys-CuS treatments.

**References**