**Electronic Supplementary Information (ESI)**

**One-pot Synthesis of Multifunctional Bi$_2$S$_3$ Nanoparticles and Construction of Core-shell Bi$_2$S$_3$@-Ce$_6$-CeO$_2$ Nanocomposites for NIR-Triggered Phototherapy**

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**Figure S1.** (a) Photothermal property of 1 mg mL$^{-1}$ Bi$_2$S$_3$ NPs aqueous dispersion when irradiated with 808 nm laser (1.5 W cm$^{-2}$). The laser was turned off after irradiation for 5 min. (b) Plot of cooling time versus negative natural logarithm of the temperature driving force obtained from the cooling stage as shown in (a). The time constant for heat transfer of the system is determined to be $\tau_s = 221.16$.

To evaluate the photothermal conversion efficiency of spheral Bi$_2$S$_3$ synthesized, the temperature change of 0.5 mL aqueous dispersion (1.0 mg mL$^{-1}$) was recorded for 5 min under continuous irradiation by the 808 nm laser with a power density of 1.5 W cm$^{-2}$, then the laser was shut off. The photothermal conversion efficiency, $\eta$, was calculated using Eq. (S1-4)

$$\eta = \frac{hS(T_{max,NPs} - T_{max,solvent})}{I(1 - 10^{-A808})}$$

(Eq.S1)
where $h$ is the heat transfer coefficient, $S$ is the surface area of the container, $T_{\text{max, NPs}}$ and $T_{\text{max, solvent}}$ are maximum steady-state temperature for Bi$_2$S$_3$ NPs solution and water, which are 31 °C and 2.2 °C, respectively. $I$ is the laser power ~ 1.5 W, and $A_{808}$ is the absorbance of Bi$_2$S$_3$ NPs at 808 nm ~ 0.335. The value of $hS$ is calculated by Eq S2:

$$\tau_s = \frac{m_D C_D}{hS} \quad \text{(Eq. S2)}$$

Where the mass of the nanoparticles solution ($m_D$) was 0.5 g, and its heat capacity ($C_D$) was approximated to be 4.2 J g$^{-1}$ k$^{-1}$ (the heat capacity of water). $\tau_s$ is the characteristic thermal time constant, which can be determined by applying the linear time data from the cooling period vs $-\ln \theta$ ($\tau_s = 221.16$, Figure S3).

$$t = \frac{\tau_s}{s} \ln(\theta) \quad \text{(Eq. S3)}$$

$$\theta = \frac{T_{\text{max, NPs}} - T_{\text{surr}}}{T_{\text{max, NPs}} - T_{\text{surr}}} \quad \text{(Eq. S4)}$$

The photothermal conversion efficiency of Bi$_2$S$_3$ NPs was calculated according to Eq. S1:

$$\eta = \frac{0.5 \times 4.2}{221.16} \times \left(31 - 2.2\right) \times 1.5 \times \left(1 - 10^{-0.335}\right) \times 100\% = 33.91\%$$

Figure S2. (a) The UV-visible absorption curve of Ce6 ethanol solution at different concentrations. (b) The UV-visible absorption standard curve of Ce6 obtained from the absorption peak at 664 nm as shown in (a). (c) The UV-visible absorption curve of 0.5 mL.
Encapsulation rate of photosensitizer Ce6
The UV-visible absorption spectrum standard curve of Ce6 at 664 nm was obtained through measuring the UV-visible absorption curve of Ce6 ethanol solution with different concentration:

\[ y = 0.0177x + 0.1315 \] (Figure S4b)

There were 3.5 mg Ce6 totally added to the Bi$_2$S$_3$ NPs solution. The UV-visible absorption peak of 0.5 mL supernatant at 664 nm was measured ~0.408 (Figure S4c), thus the concentration of Ce6 in supernatant is calculated:

\[ \frac{0.408 - 0.1315}{0.0177} = 15.6 \]

There were 34 mL supernatant collected, thus the amount of Ce6 unencapsulated into Bi$_2$S$_3$ NPs was obtained: 15.6 μg × 34 = 1.06 mg. The encapsulation rate \( \varphi \) of Ce6 was calculated according to:

\[ \varphi = \frac{Ce6_{total \ amount} - Ce6_{supernatant}}{Ce6_{total \ amount}} \times 100\% = \frac{3.5 - 1.06}{3.5} \times 100\% = 69.7\% \]

Figure S3. (a) the energy spectrum analysis of two points in Bi$_2$S$_3$@Ce6-CeO$_2$ NCs (b) the HRTEM image of Bi$_2$S$_3$@Ce6-CeO$_2$ NCs.
Figure S4. (a) Photothermal property of 1 mg mL\(^{-1}\) Bi\(_2\)S\(_3\)@-Ce6-CeO\(_2\) NCs aqueous dispersion when irradiated with 808 nm laser (1.5 W cm\(^{-2}\)). The laser was turned off after irradiation for 5 min. (b) Plot of cooling time versus negative natural logarithm of the temperature driving force obtained from the cooling stage as shown in (a). The time constant for heat transfer of the system is determined to be \(\tau_s = 205.36\).

To evaluate the photothermal conversion efficiency of Bi\(_2\)S\(_3\)@-Ce6-CeO\(_2\) NCs, the temperature change of 0.5 mL aqueous dispersion was recorded for 5 min under continuous irradiation by the 808 nm laser with a power density of 1.5 W cm\(^{-2}\), then the laser was shut off. The photothermal conversion efficiency, \(\eta\), was calculated using Eq. (S1-4):

\[
\eta = \frac{hS(T_{\text{max, NPs}} - T_{\text{max, solvent}})}{I(1 - 10^{-A_{808}})}
\]

where \(h\) is the heat transfer coefficient, \(S\) is the surface area of the container, \(T_{\text{max, NPs}}\) and \(T_{\text{max, solvent}}\) are maximum steady-state temperature for Bi\(_2\)S\(_3\)@-Ce6-CeO\(_2\) NCs solution and water, which are 32.9 °C and 2.2 °C, respectively. \(I\) is the laser power \(\sim 1.5\) W, and \(A_{808}\) is the absorbance of Bi\(_2\)S\(_3\)@-Ce6-CeO\(_2\) NCs at 808 nm \(\sim 0.597\). The value of \(hS\) is calculated by Eq2:

\[
\tau_s = \frac{m_DC_D}{hS}
\]

Where the mass of the nanoparticles solution \((m_D)\) was 0.5 g, and its heat capacity \((C_D)\) was approximated to be 4.2 J g\(^{-1}\) k\(^{-1}\) (the heat capacity of water). \(\tau_s\) is the characteristic thermal time constant, which can be determined by applying the linear time data from the cooling period vs \(-\ln \theta\) (\(\tau_s = 205.36\)).

\[
t = \tau_s \ln(\theta)
\]

\[
\frac{T - T_{\text{surr}}}{T_{\text{max, NPs}} - T_{\text{surr}}} = \frac{1}{\tau_s} \ln(\theta)
\]

The photothermal conversion efficiency of Bi\(_2\)S\(_3\)@-Ce6-CeO\(_2\) NCs was calculated according to Eq. 1:
\[
\eta = \frac{0.5 \times 4.2 \times (33.9 - 2.2)}{205.36 \times 1.5 \times (1 - 10^{-0.597})} \times 100\% = 28.01\%
\]

Figure S5. ΔT curves of (a) Bi\(_2\)S\(_3\)@Ce6-CeO\(_2\) NCs aqueous solution of various concentrations after 5 min irradiation of 808 nm NIR laser (1.5 W cm\(^{-2}\)). (b) Bi\(_2\)S\(_3\)@Ce6-CeO\(_2\) NCs aqueous solution with 808 nm NIR laser irradiating and then self-cooling for 3 cycles.

Figure S6. the production of \(^1\)O\(_2\) in 4T1 cells after incubation with Bi\(_2\)S\(_3\)@Ce6-CeO\(_2\) NCs at 200 μg mL\(^{-1}\) and then get a 660 nm laser’s illumination of different light power (0, 110, 200
mW) for two minutes. Scale bar: 100 μm

![Diagram](image1)

**Figure S7.** (a) Standard curve of H$_2$O$_2$ concentration measured by H$_2$O$_2$ standard kit H$_2$O$_2$ consumption. (b) Curve of H$_2$O$_2$ concentration in 4T1 cells after incubating with a series of different concentrations of Bi$_2$S$_3$@Ce6-CeO$_2$ and Bi$_2$S$_3$@Ce6 (0, 12.5, 25, 50, 100 and 200 μg mL$^{-1}$) by H$_2$O$_2$ detection kit.

![Diagram](image2)

**Figure S8.** The percentage of TUNEL positive cancer cells after getting saline, 660/808 nm, NCs, NCs + 660 nm, NCs + 808 nm and NCs + 660/808 nm treatment, respectively (ns means no statistical difference compared with the control group. *p<0.05, **p<0.01 and ***p<0.001 compared with the control group).
Figure S9. Representative H&E staining of heart, liver, spleen, lung, and kidney from saline, 660/808 nm, NCs, NCs + 660 nm, NCs + 808 nm and NCs + 660/808 nm treated rats. The percentage of TUNEL positive cancer cells after various treatments. Scale bar: 100 μm.