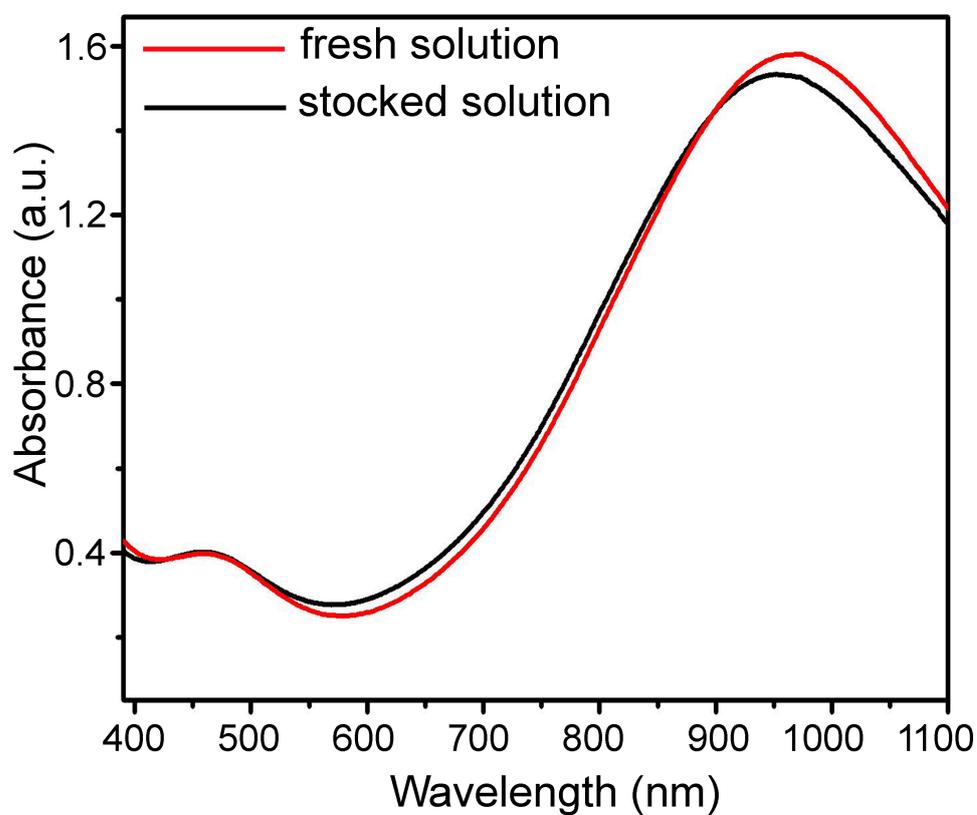


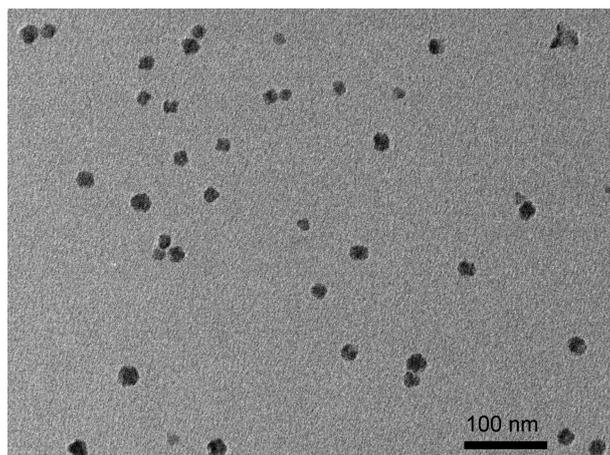
## Electronic Supplementary Information

### **Cu<sub>7.2</sub>S<sub>4</sub> Nanocrystals: A Novel Photothermal Agent with a 56.7% Photothermal Conversion Efficiency for Photothermal Therapy of Cancer Cells**

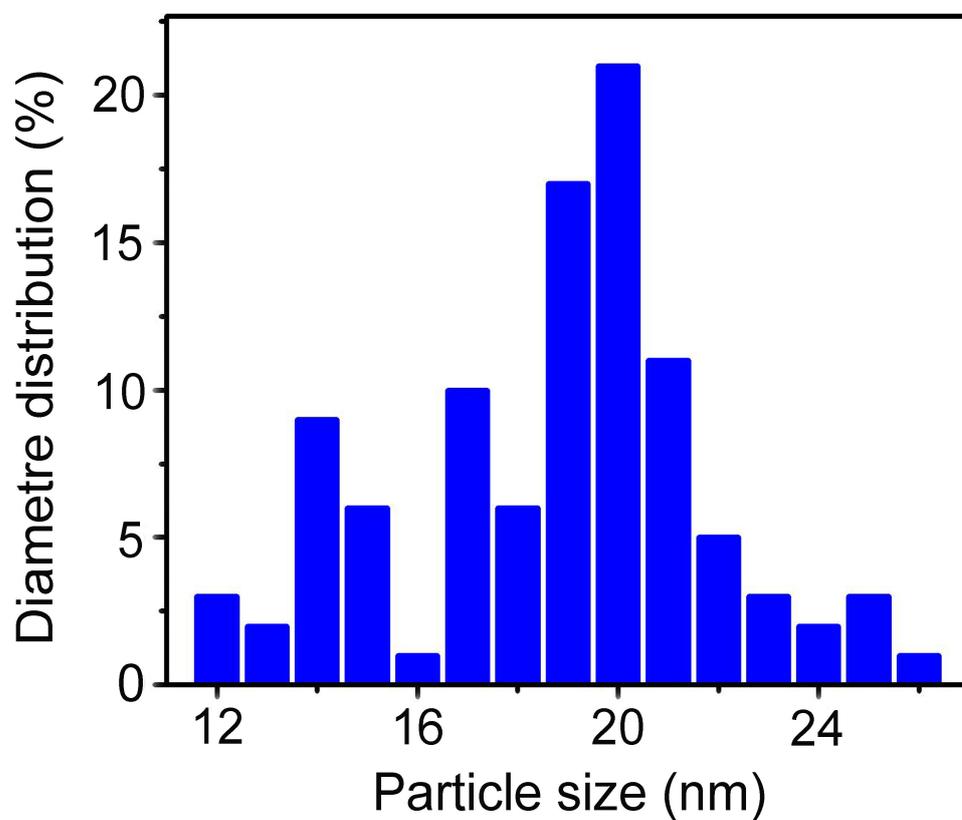
Bo Li,<sup>a</sup> Qian Wang,<sup>ab</sup> Rujia Zou,<sup>a</sup> Xijian Liu,<sup>a</sup> Kaibing Xu,<sup>a</sup> Wenyao Li,<sup>a</sup> and Junqing Hu<sup>\*a</sup>



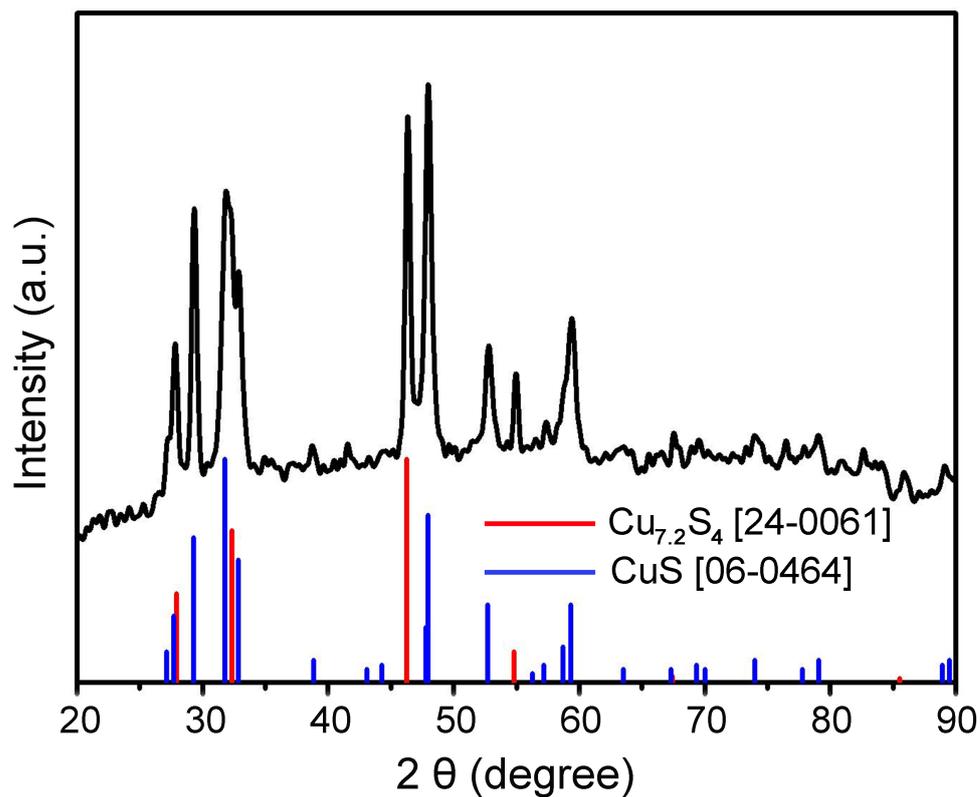
**Fig. S1** UV-vis spectra of the freshly prepared Cu<sub>7.2</sub>S<sub>4</sub> NCs and the Cu<sub>7.2</sub>S<sub>4</sub> NCs stocked in chloroform under ambient conditions for 2 months.



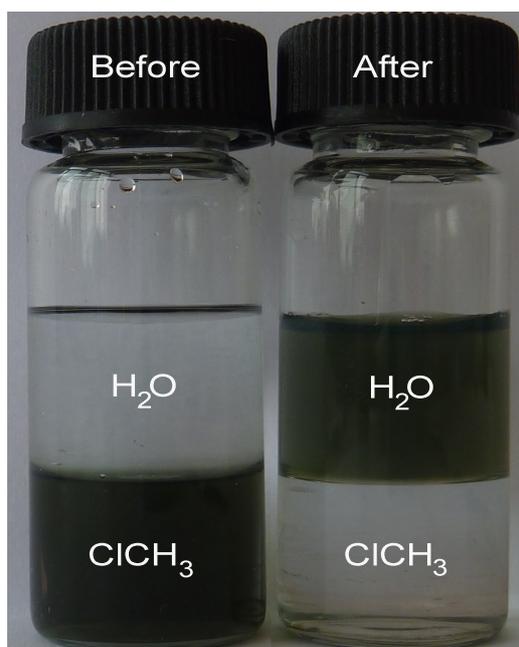
**Fig. S2** TEM image of Cu<sub>7.2</sub>S<sub>4</sub> NCs stocked in chloroform for two months.



**Fig. S3** Histogram showing the size distribution of the Cu<sub>7.2</sub>S<sub>4</sub> NCs.

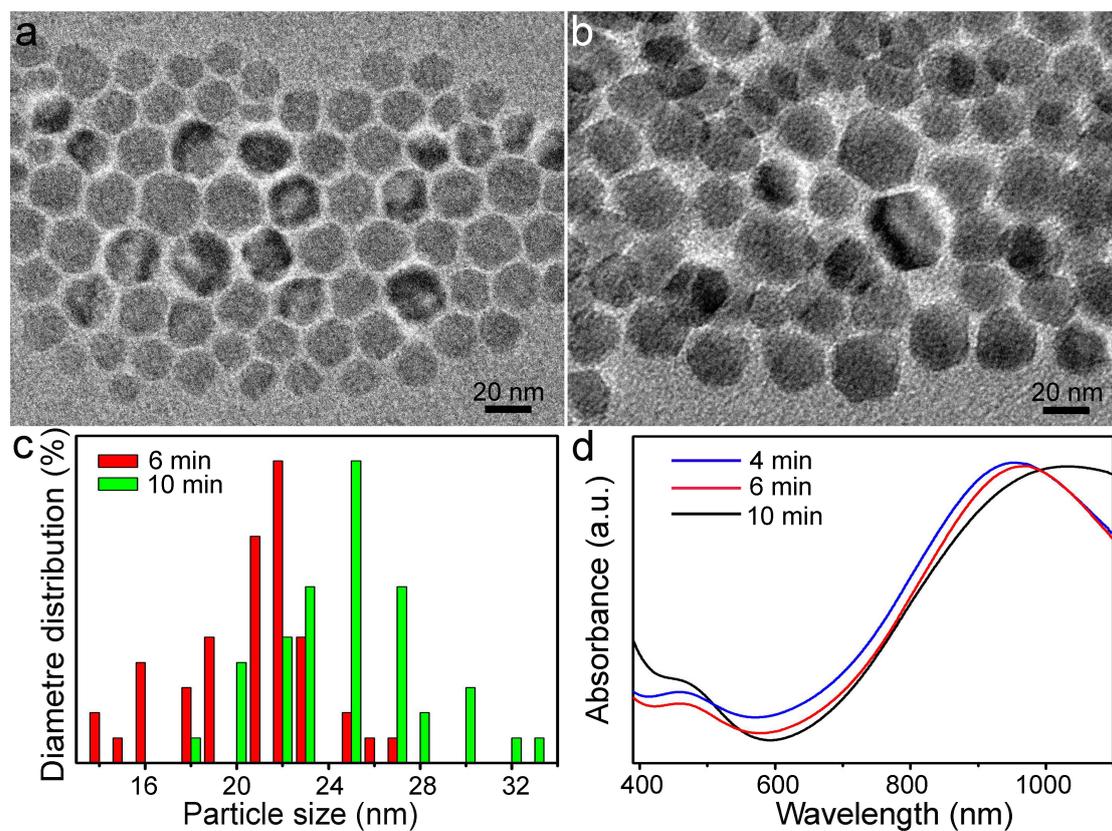


**Fig. S4** XRD patterns of the product obtained under injection temperature below 240 °C

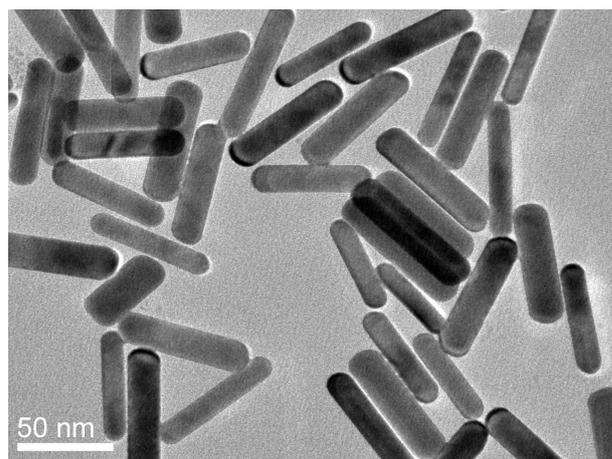


**Fig. S5** A digital camera photo showing the  $\text{Cu}_{7.2}\text{S}_4$  NCs dispersed into different

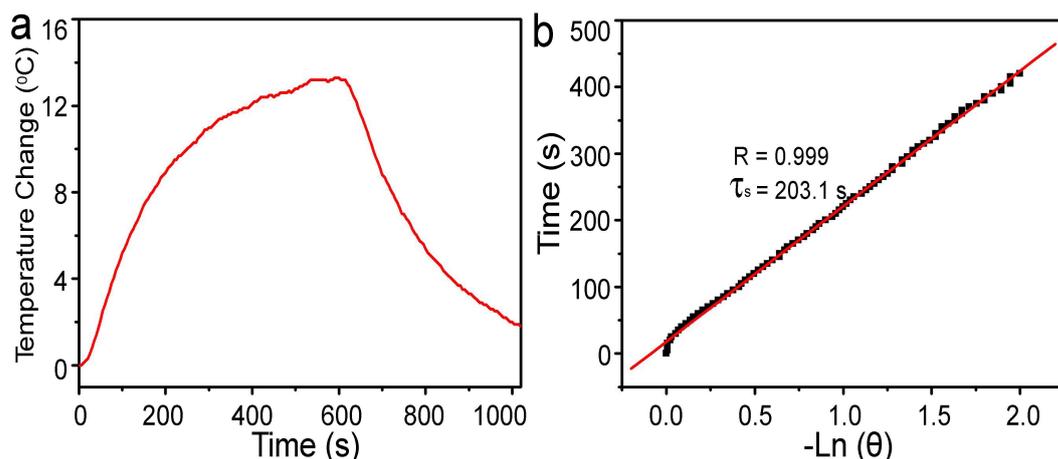
solvents ( $\text{H}_2\text{O}$  and  $\text{CHCl}_3$ ) before and after the polymer coating.



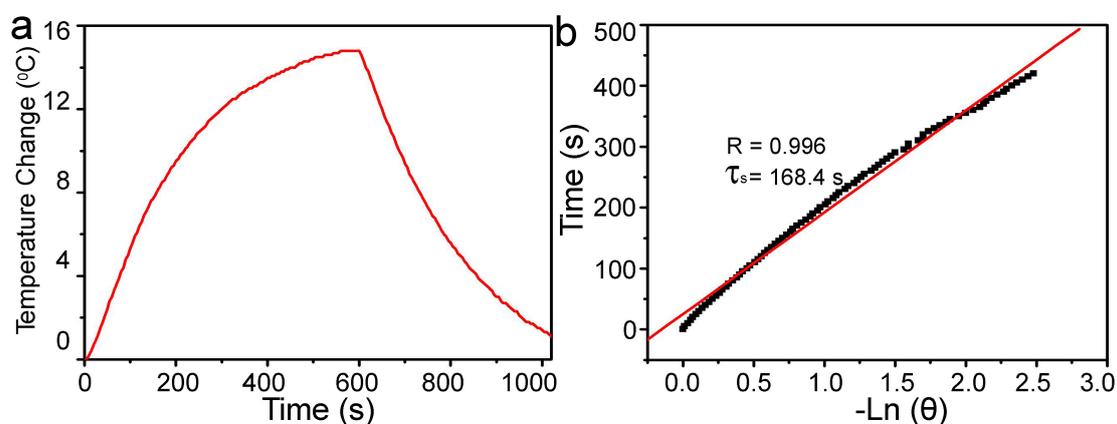
**Fig. S6** TEM images of the  $\text{Cu}_{7.2}\text{S}_4$  NCs collected via 6 min a) and 10 min b); c) Histogram showing the size distribution of the  $\text{Cu}_{7.2}\text{S}_4$  NCs from S6a and S6b; d) UV-vis spectra of the  $\text{Cu}_{7.2}\text{S}_4$  NCs collected via different time.



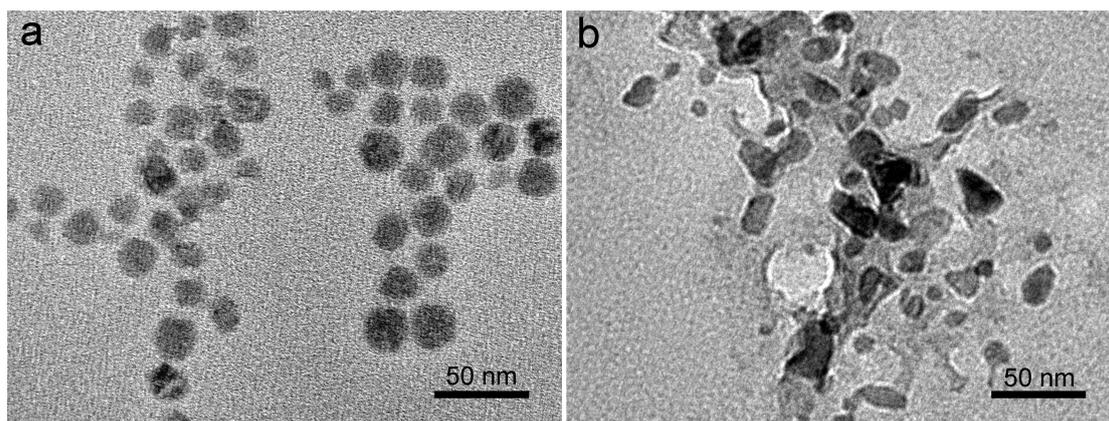
**Fig. S7** TEM image of the CTAB capped Au nanorods



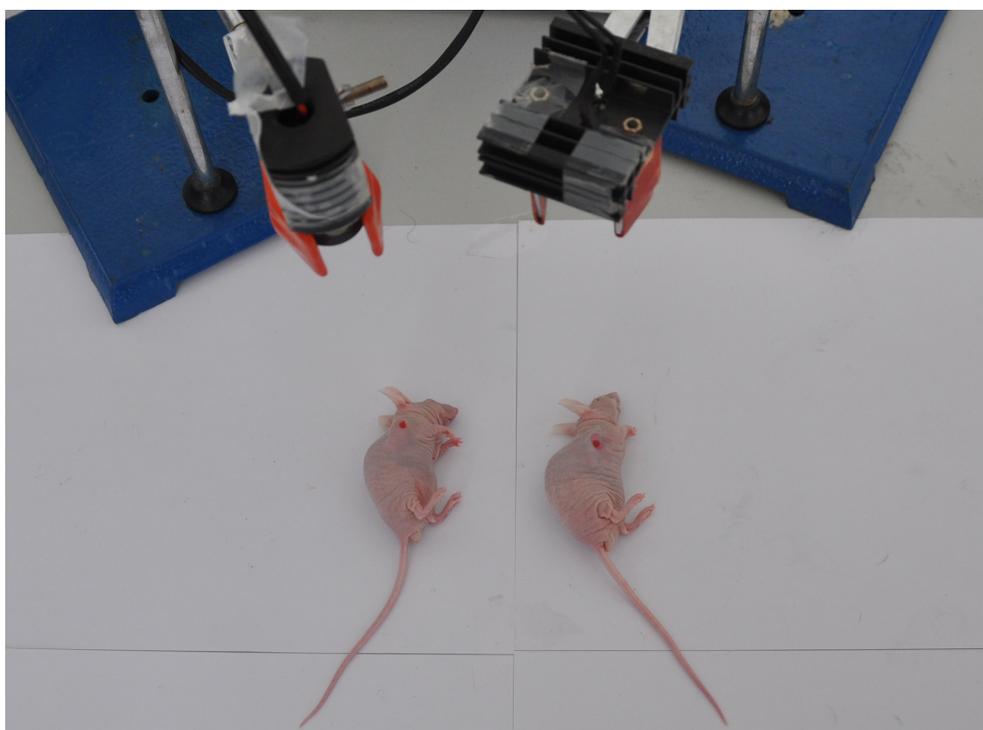
**Fig. S8** a) Photothermal effect of 40 ppm Au nanorods upon being irradiated for 10 min (980 nm, 0.29 W) and shutting off the laser. b) Time constant for heat transfer from the system is determined to be  $\tau_s = 203.1$  s by applying the linear time data from the cooling period of Figure S6a versus negative natural logarithm of driving force temperature.



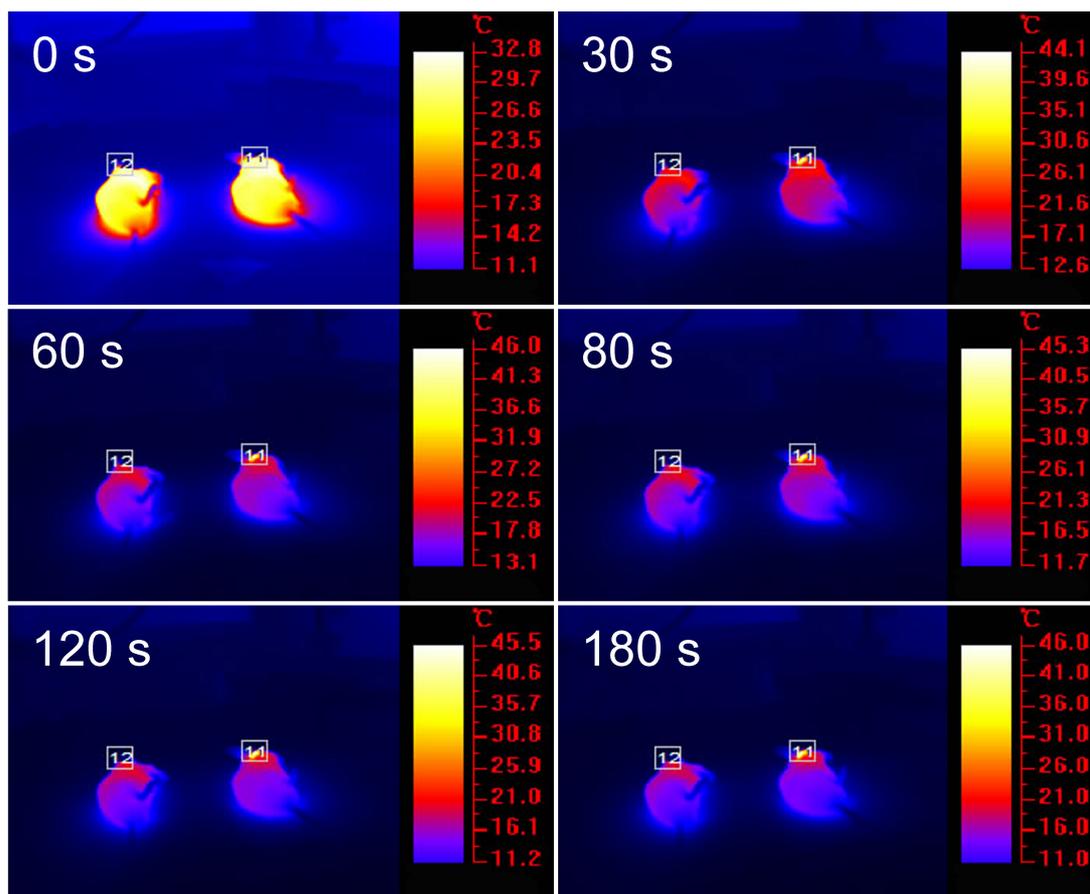
**Fig. S9** a) Photothermal effect of 40 ppm Au nanorods upon being irradiated for 10 min (808 nm, 0.29 W) and then shutting off the laser. b) Time constant for heat transfer from the system is determined to be  $\tau_s = 168.4$  s by applying the linear time data from the cooling period of Fig. S9a versus negative natural logarithm of driving force temperature.



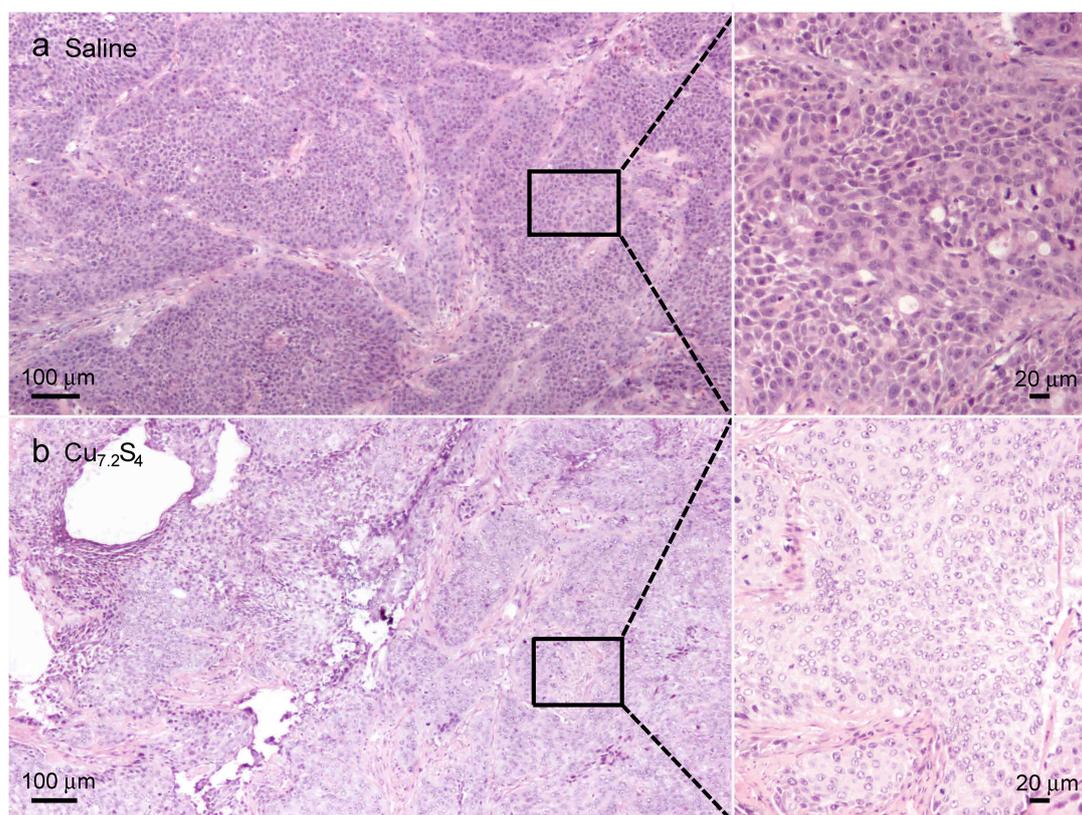
**Fig. S10 TEM images of Cu<sub>7.2</sub>S<sub>4</sub> NCs (a) and Au nanorods (b) after four LASER ON/OFF cycles of NIR light (980 nm, 2W) irradiation**



**Fig. S11** Photograph showing the typical experimental setup for in vivo photothermal therapy of cancer cells.



**Fig. S12** The full-body thermographic images of mice containing tumors which were injected with saline solution (left mouse, indicated region 12) and PBS solution containing  $\text{Cu}_{7.2}\text{S}_4$  NCs (right mouse, indicated region 11), under the irradiation of 980-nm laser with the safe density of  $0.72 \text{ Wcm}^{-2}$  for different time (0-180 s).



**Fig. S13** Representative H & E stained histological images of *ex vivo* tumor sections injected with: a) saline and b) an aqueous dispersion of Cu<sub>7.2</sub>S<sub>4</sub> NCs (40 ppm), respectively. The sections were irradiated with the 980-nm laser irradiation with the safe density of 0.72 Wcm<sup>-2</sup> for 7 min.