Electronic Supplementary Material (ESI) for Nanoscale.

PEGylated Nickel Carbide Nanocrystals as Efficient Near-Infrared Laser Induced Photothermal Therapy for Treatment of Cancer Cells *In Vivo*

Zhiguo Zhou[a], Jun Wang[a], Wei Liu[a], Chao Yu[a], Bin Kong[a], Yanan Sun[a], Hong Yang[a], Shiping Yang[a]* and Wei Wang[a, b]*

[a] *The Education Ministry Key Lab of Resource Chemistry and Shanghai Key Laboratory of Rare Earth Functional Materials, Shanghai Normal University, Shanghai 200234, China*

[b] *Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, New Mexico 87131-000*

Corresponding author：

Fax: 86-21-64322346; Tel: 86-21-64322346.

Email: shipingy@shnu.edu.cn (S. P. Yang) and wwang@unm.edu (W. Wang)

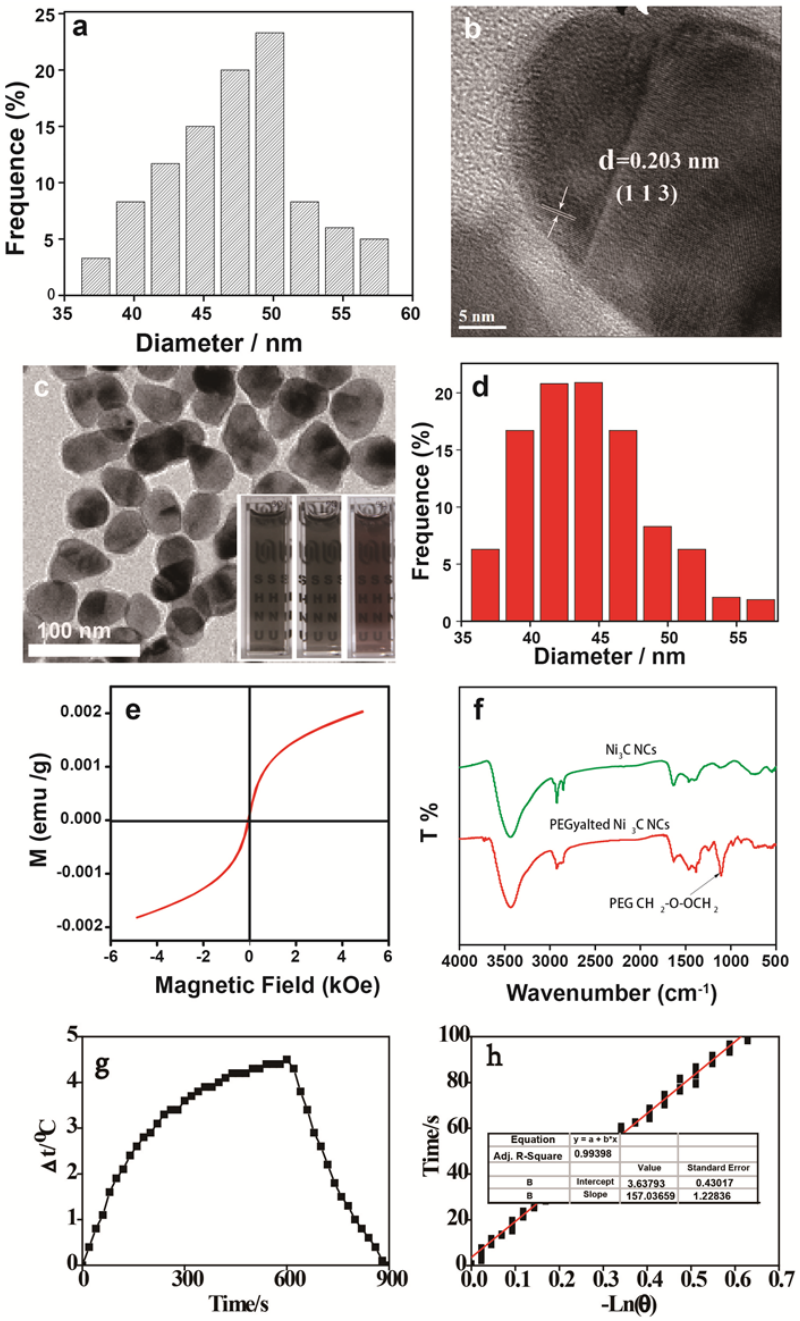

Fig. S1 TEM image of PEGylated Ni_3C NCs and the photograph in water (2 mg/mL, inset) (a). Inset: Photograph of PEGylated Ni_3C NCs (200 μg/mL) in water (left), PBS (middle) and RMPI-1640 plus 10% FBS (right). HRTEM image of Ni_3C NCs (b). Size distribution of Ni_3C NCs (c) and PEGylated Ni_3C NCs (d). The hysteresis loop of Ni_3C NCs (e). FT-IR spectra of Ni_3C NCs and PEGyalted Ni_3C NCs (f). Cyclic curve of the aqueous solution of PEGylated Ni_3C NCs (100 μg/mL) under the 808 nm laser irradiation with a power density of 1 W/cm^2 (g). Linear time data versus −lnθ obtained from the cooling period (h). The conversion efficiency (16.9%) was measured using the literature reported protocol (Y. Liu, K. Ai, J. Liu, M. Deng, Y. He, L. Lu, *Adv. Mater.* 2013, **25**, 1353-1359). The aqueous solution of PEGylated Ni_3C NCs (100 μg/mL, 1 mL) was put in a quartz cuvette with an optical path of 1 cm, then exposed to the 808 nm laser with a power density of 1 W/cm^2 for 10 min, then the laser was turned off. The diameter of the laser spot was 1 cm. The temperature was recorded by FLIR A300 (USA).

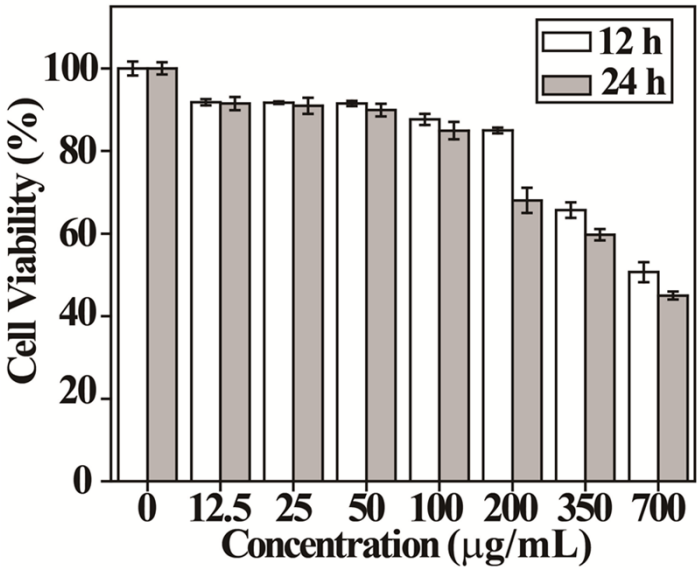

Fig. S2 Cell viability of HeLa cells incubated with different concentrations of PEGylated Ni_3C NCs in the saline solution (0-700 μg/mL) for 12 and 24 h, respectively.

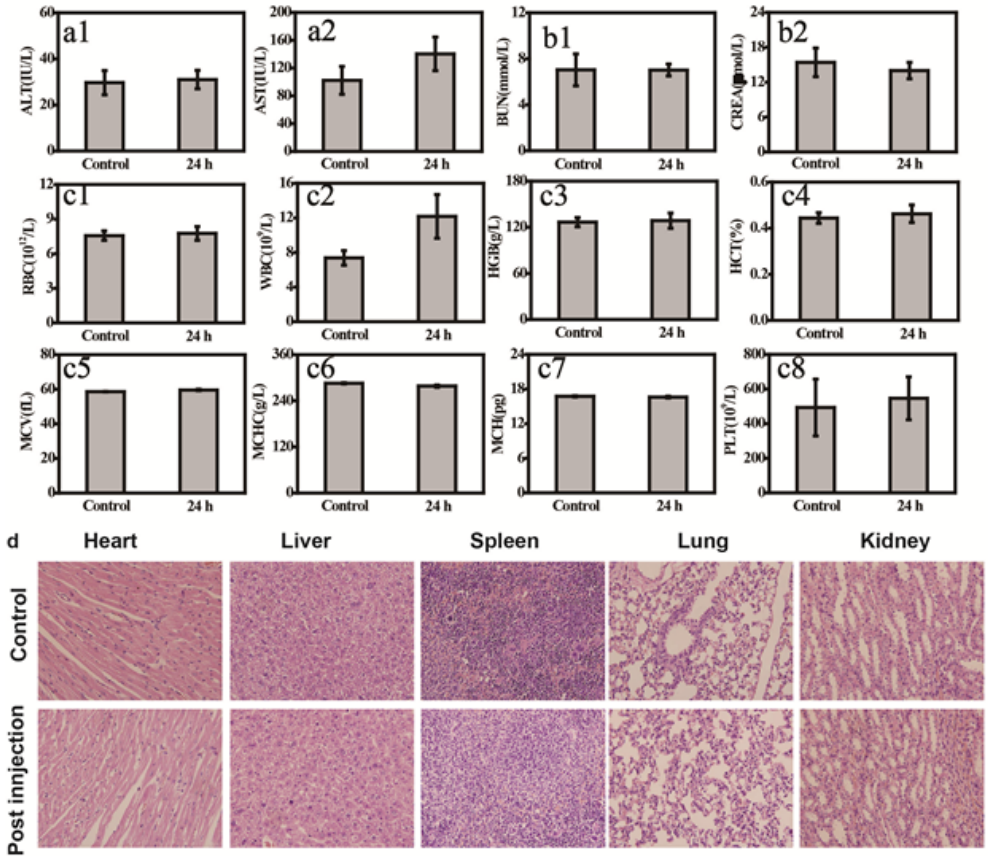

Fig. S3 Blood analysis data of ICR rats intravenously injected with PEGylated Ni_3C NCs (10 mg·kg^{-1} body weight) in a saline solution. Untreated rats were used as the control groups. Liver function index includes alanine aminotransferase (ALT, a1) and aspartate aminotransferase (AST, a2). Kidney function index includes urea nitrogen (BUN, b1) and creatinine (CREA, b2). The complete blood analysis includes red blood cells (RBC, c1), white blood cells (WBC, c2), haemoglobin (HGB, c3), hematocrit (HCT, c4), mean corpuscular volume (MCV, c5) mean corpuscular hemoglobin concentration (MCHC, c6), mean corpuscular hemoglobin (MCH, c7) and platelets (PLT, c8). Statistics were based on three mice per data point. (d) Histological changes in the heart, liver, spleen, lung and kidney of ICR rats without and with intravenous injection of PEGylated Ni_3C NCs (10 mg·kg^{-1} body weight) after 24 h. These organs were stained with H&E and observed under a light microscope at 40 × magnification.

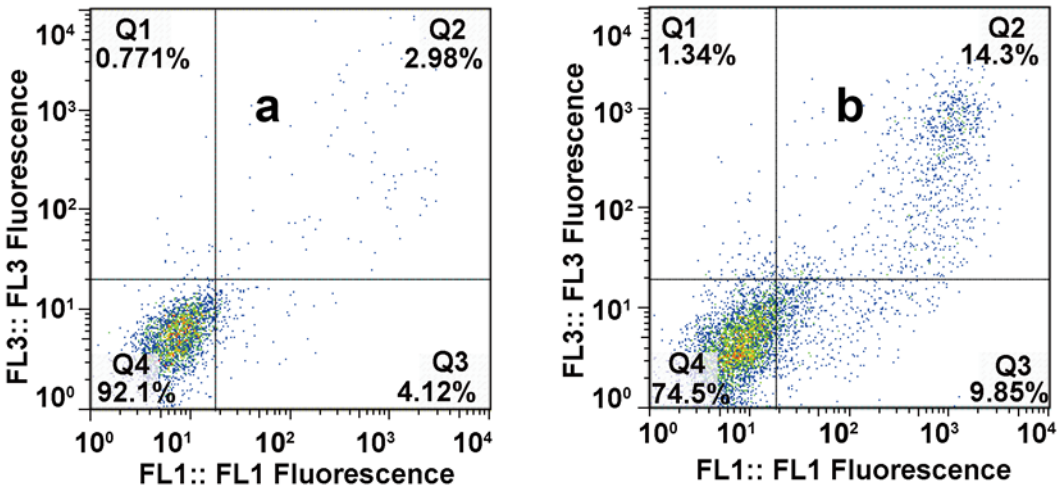

Fig. S4 Representative FACS plots of HeLa cells after an 808 nm laser irradiation for 10 min (0.25 W/cm^2) (a) and incubated with 50 μg/mL PEGylated Ni_3C NCs in a saline solution after an 808 nm laser irradiation for 10 min (0.25 W/cm^2) (b).

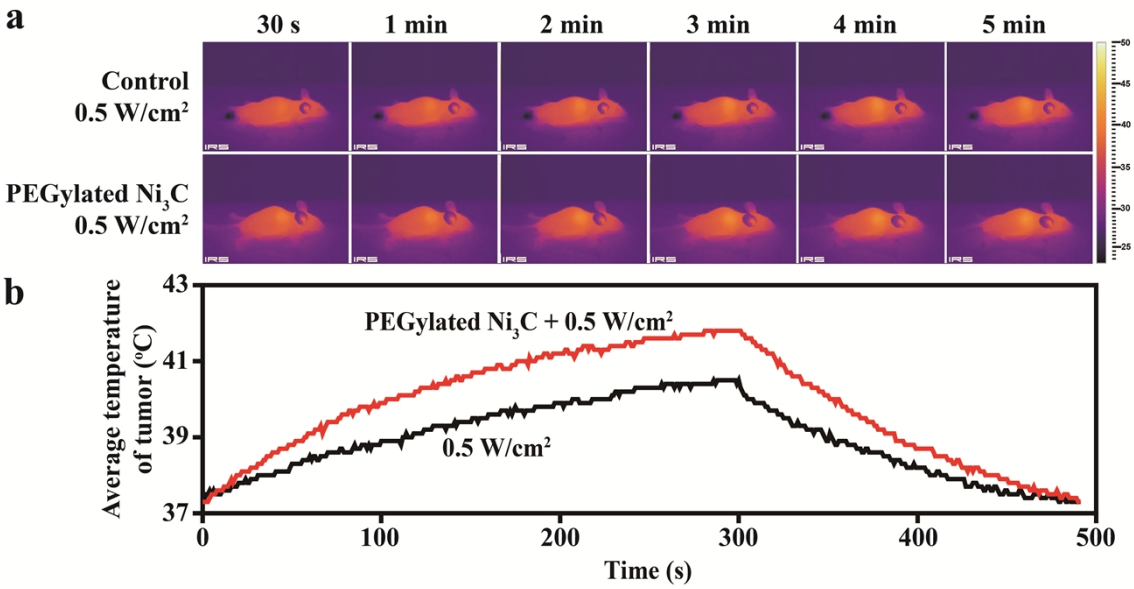

Fig. S5 (a) Thermal infrared images of tumor area intravenously injected with PEGylated Ni_3C NCs (10 mg·kg^{-1}) in a saline solution recorded at different time intervals. Mice injected saline was taken as the control group. The tumor was exposed to an 808 nm laser with a power density of 0.25 and 0.5 W/cm^2, respectively. (b) Plots of tumor temperature as a function of time which corresponded to (a).

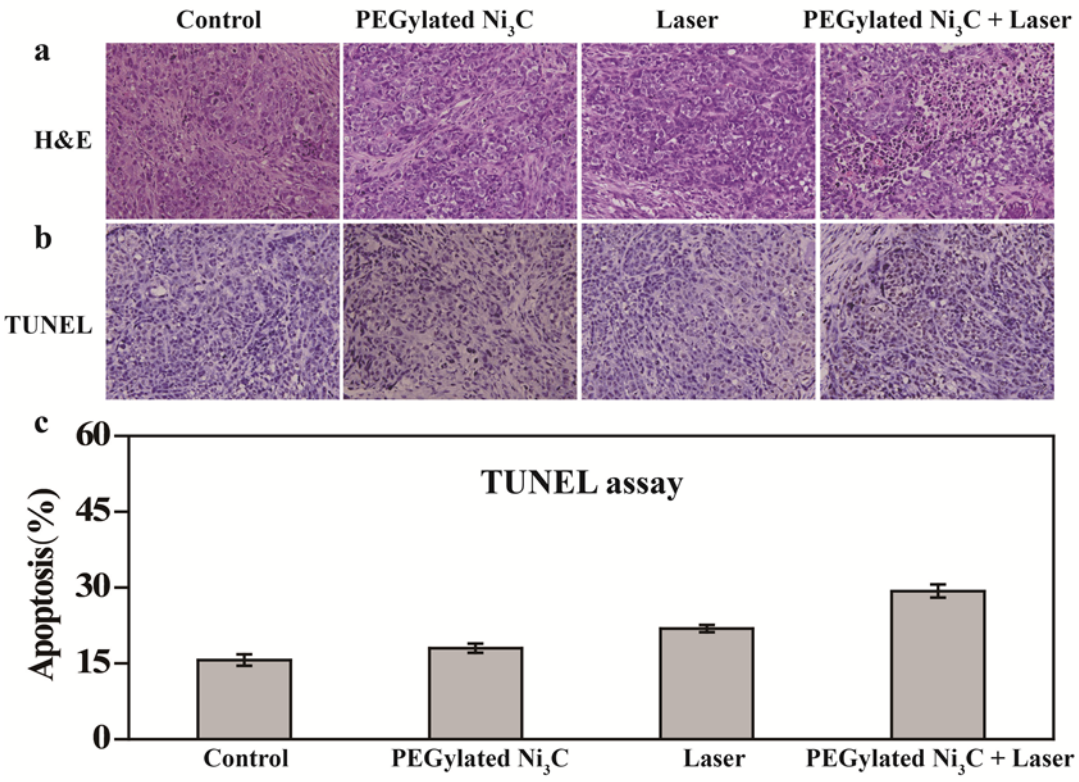

Fig. S6 H&E (a) and TUNEL (b) stained histological images of tumor sections. (c) The percentage of TUNEL-positive cells in tumor sections with different experiment groups.

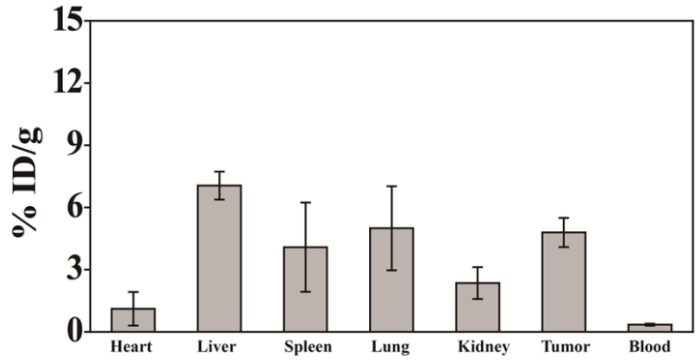

Fig. S7 Biodistribution of PEGylated Ni_3C NCs in HeLa tumor-bearing mice determined by ICP-AES.