Supplementary Data

Targeted Photothermal Therapy on Mice and Rabbit: Realized by Macrophage Loaded Tungsten Carbide

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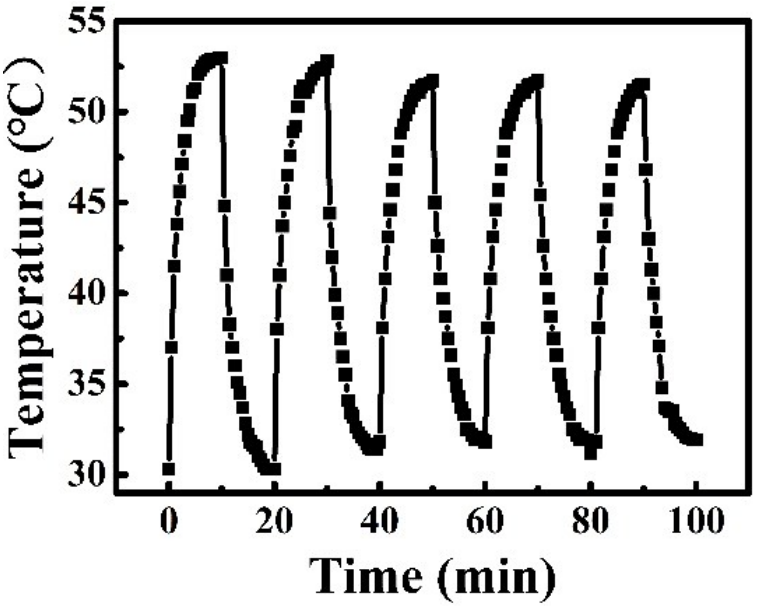

Fig. S1. Temperature curve of M-WC aqueous dispersion with repeated irradiation on/off cycles (880 nm, 1 W cm^{-2}).

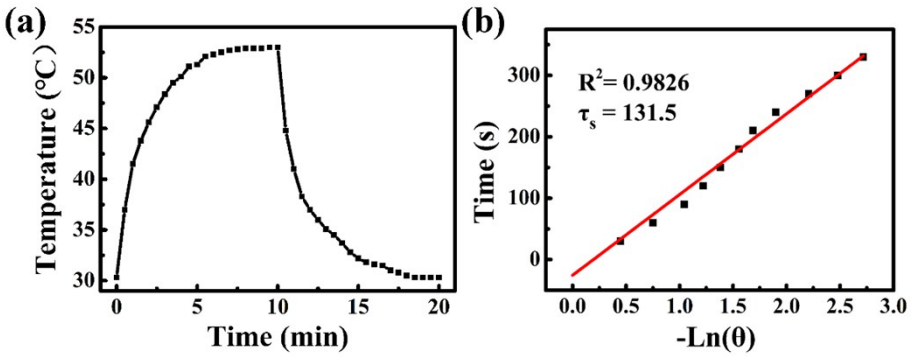

Fig. S2. (a) Temperature curve of the M-WC (0.5 mg/mL) dispersion under NIR irradiation and after removing the NIR, (b) the curve of - Ln(θ) versus Time.

To further assess the photothermal performance of M-WC, the photothermal conversion efficiency (η) was quantified according to following eqution.[S1,S2]

$$\eta = [hS\,(T_{max} - T_{surr}) - Q_{dis}]/\,I(1-10^{-A_{880}}) \qquad \textbf{Equation S1}$$

where h is heat transfer coefficient, S is the surface area of the container, T_{max} is the equilibrium temperature (53 ℃), T_{surr} is ambient temperature of the surroundings (31.1 ℃), Q_{dis} is heat dissipated from light absorbed by the quartz sample cell itself (11.34 mW), I is incident laser power (1 W cm^{-2}), A_{880} is the optical absorbance of nanoparticles at 880 nm (1.452).

In order to obtain the value of hS, a dimensionless driving force temperature θ was introduced:

$$\Theta = (T-T_{surr})/(T_{max}-T_{surr}) \qquad \textbf{Equation S2}$$

M-WC were continuously irradiated for 10 min, followed by natural cooling to room temperature for 10 min. According to the cooling curve in **Figure R3a**, the curve of - Ln(θ) versus time were obtained (**Figure R3b).** The cooling time t and θ abide by the following equation S3:

$$t = -\tau_s \ln(\Theta) \qquad \textbf{Equation S3}$$

In this way, the time constant (τ_s) was calculated to be 131.5s.

The value of hS can be calculated by the following equation:

$$hS = \Sigma mCp/\tau s \qquad \textbf{Equation S4}$$

Where **m** is the mass (0.5 g), Cp is heat capacity of water (4.2 J/g) and $\boldsymbol{\tau_s}$ is time constant, respectively. Thus, the photothermal conversion efficiency value was determined to be 25.8%.

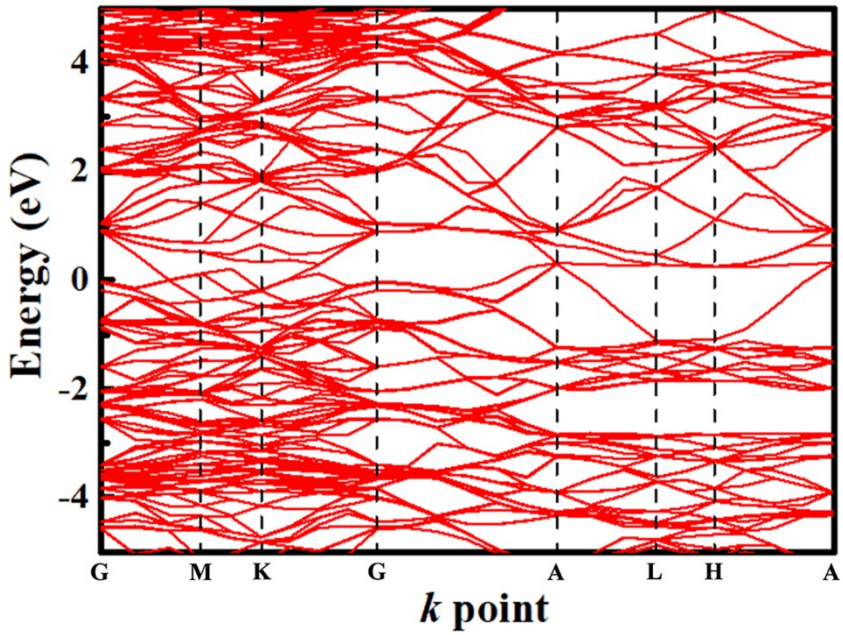

Fig. S3. Band structure was calculated along the specific path: G-M-K-G-A-L-H-A of WC hexagonal lattice.

Table S1. The DFT calculated atomic Mulliken populations.

Atom Species	s	p	d	Net Charge (e)
C1	1.38	3.22	0	-0.6
C2	1.38	3.22	0	-0.6
C3	1.38	3.22	0	-0.6
C4	1.38	3.22	0	-0.6
C5	1.38	3.22	0	-0.6
C6	1.38	3.22	0	-0.6
C7	1.38	3.22	0	-0.6
C8	1.38	3.22	0	-0.61
C9	1.38	3.22	0	-0.6
C10	1.38	3.22	0	-0.6
C11	1.38	3.22	0	-0.6
C12	1.38	3.22	0	-0.6
C13	1.38	3.22	0	-0.6
C14	1.38	3.22	0	-0.6
C15	1.38	3.22	0	-0.6
C16	1.38	3.22	0	-0.61
C17	1.38	3.22	0	-0.6
C18	1.38	3.22	0	-0.6
C19	1.38	3.22	0	-0.6
C20	1.38	3.22	0	-0.6
C21	1.38	3.22	0	-0.6
C22	1.38	3.22	0	-0.6
C23	1.38	3.22	0	-0.6
C24	1.38	3.22	0	-0.6
C25	1.38	3.22	0	-0.6
C26	1.38	3.22	0	-0.6
C27	1.38	3.22	0	-0.6
C28	1.38	3.22	0	-0.6
C29	1.38	3.22	0	-0.6
C30	1.38	3.22	0	-0.6
C31	1.38	3.22	0	-0.6
C32	1.38	3.22	0	-0.6
W1	2.46	6.53	4.41	0.61

W2	2.46	6.53	4.41	0.6
W3	2.46	6.53	4.41	0.61
W4	2.46	6.53	4.41	0.6
W5	2.46	6.53	4.41	0.61
W6	2.46	6.53	4.41	0.6
W7	2.46	6.53	4.41	0.6
W8	2.46	6.53	4.41	0.61
W9	2.46	6.53	4.41	0.61
W10	2.46	6.53	4.41	0.6
W11	2.46	6.53	4.41	0.6
W12	2.46	6.53	4.41	0.6
W13	2.46	6.53	4.41	0.6
W14	2.46	6.53	4.41	0.6
W15	2.46	6.53	4.41	0.6
W16	2.46	6.53	4.41	0.61
W17	2.46	6.53	4.41	0.6
W18	2.46	6.53	4.41	0.61
W19	2.46	6.53	4.41	0.6
W20	2.46	6.53	4.41	0.6
W21	2.46	6.53	4.41	0.61
W22	2.46	6.53	4.41	0.6
W23	2.46	6.53	4.41	0.6
W24	2.46	6.53	4.41	0.6
W25	2.46	6.53	4.41	0.6
W26	2.46	6.53	4.41	0.61
W27	2.46	6.53	4.41	0.61
W28	2.46	6.53	4.41	0.6
W29	2.46	6.53	4.41	0.61
W30	2.46	6.53	4.41	0.6
W31	2.46	6.53	4.41	0.6
W32	2.46	6.53	4.41	0.6

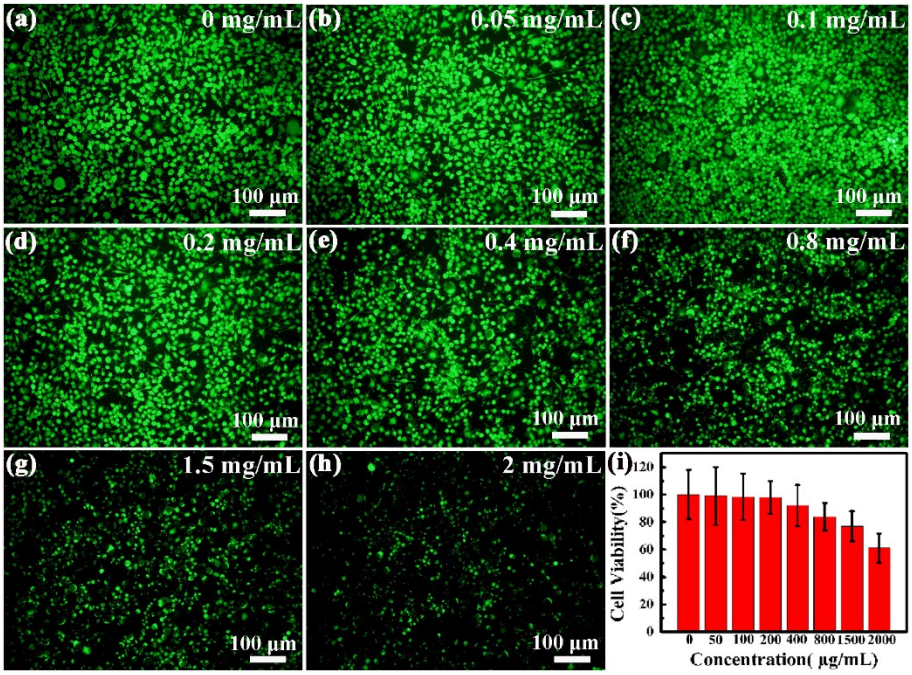

Fig. S4. (a) - (h) Calcien AM staining for the observation of living macrophage after incubation with viaried concentration of WC, (i) Relative cell viability after treated with various concentrations of M-WC.

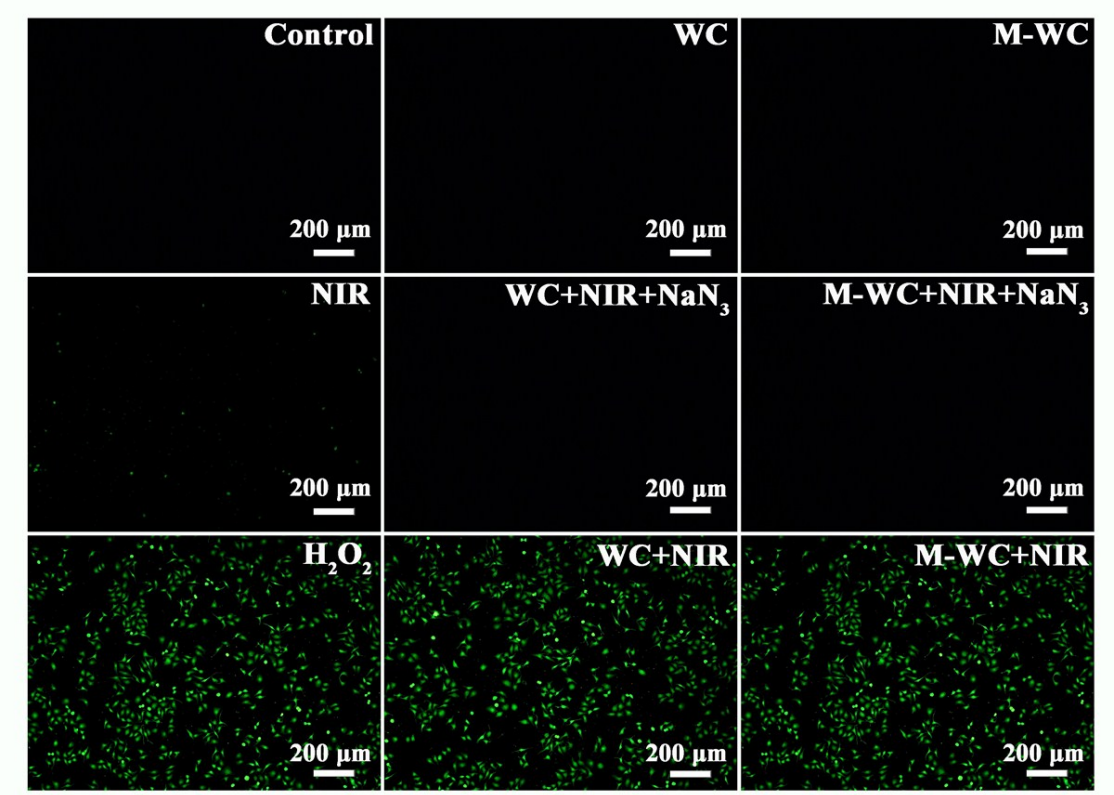

Fig. S5. Fluorescence microscope images of ROS generation determined by the H2DCFDA probe.

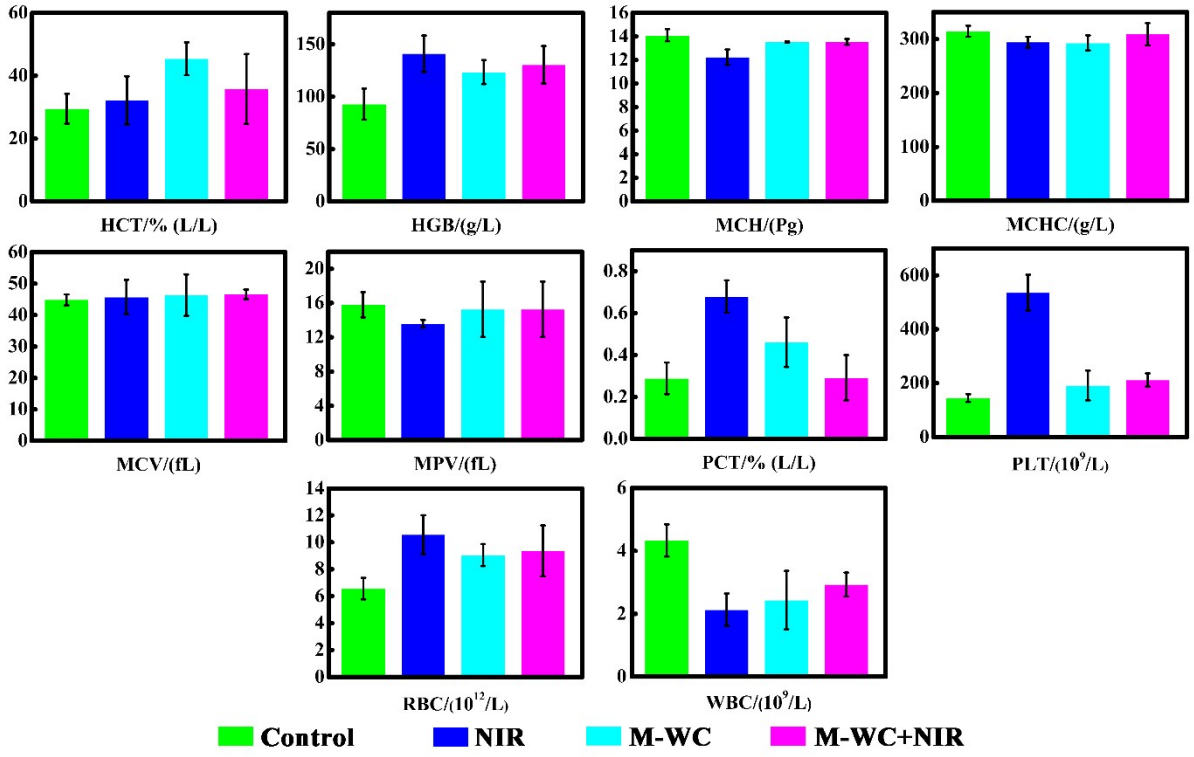

Fig. S6. Hemanalysis results of all the mice in different groups.

References

S1. M. F. Wang, K. R. Deng, W. Lu, X. R. Deng, K. Li, Y. S. Shi, B. B. Ding, Z. Y. Cheng, B. G. Xing, G. Han, Z. Y. Hou and J. Lin, *Adv. Mater.*, 2018, **30**, 1706747.

S2. C. B. Leng, X. Zhang, F. X. Xu, Y. Yuan, H. Pei, Z. H. Sun, L. Li and Z. H. Bao, *Small*, 2018, **14**, 1703077.