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Supporting Information for

2D Magnetic Titanium Carbide (MXene) for Cancer Theranostics

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Calculation of the extinction coefficient

According to the Lambert-Beer law (1), the extinction coefficient $\alpha(\lambda)$ of Ti_3C_2-IONPs-SPs nanocomposites is obtained.

$$A(\lambda)/L=\alpha C \quad (1)$$

A means the absorbance at a wavelength λ, α means the extinction coefficient, L means path-length (1 cm), and C means the concentration of the Ti_3C_2-IONPs-SPs nanocomposites (g L^{-1}). The extinction coefficient α is determined by plotting the slope (in L g^{-1} cm^{-1}) of each linear fit against wavelength.

Calculation of the photothermal-conversion efficiency

According to the previous report,[2] the energy balance for the system is

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = Q_{Ti3C2-IONPs-SPs} + Q_{Dis} - Q_{surr} \quad (2)$$

M and C_p mean the mass and heat capacity of deionized water, T means temperature of solution, $Q_{Ti3C2-IONPs-SPs}$ means the heat dissipated by electron-phonon relaxation of the plasmon on the surface of Ti_3C_2-IONPs-SPs irradiated under 808 nm laser, Q_{Dis} means the heat dissipated from light absorbed by the sample cell itself, and Q_{surr} means the heat conduction from surrounding.

$$Q_{Ti3C2-IONPs-SPs} = I\,(1\text{-}10^{-A808})\,\eta \quad (3)$$

I means the laser power (mW), A_{808} means the absorbance of Ti_3C_2-IONPs-SPs at the excitation wavelength of 808 nm, and η means the photothermal conversion efficiency which we aim to obtain.

Q_{Dis} means the heat dissipated from light absorbed by the sample cell itself and it is measured independently to be 5.4×10^{-4} I mW.

$$Q_{surr} = hS\,(T\text{-}T_{surr}) \quad (4)$$

h means the heat transfer coefficient, S means the surface area of the cell, and T_{surr} means the ambient surrounding temperature. When the laser power is irradiated, heat input

($Q_{Ti3C2-IONPs-SPs} + Q_{Dis}$) will be finite. As the heat output Q_{surr} is increased along with the temperature according to the equation (4), the temperature of the whole system will rise to the maximum when the heat input equivalent to the heat output.

$$Q_{Ti3C2-IONPs-SPs} + Q_{Dis} = Q_{surr-max} = hS\,(T_{max}\text{-}T_{surr}) \quad (5)$$

$Q_{surr-max}$ means the heat condition away from the system when the Ti_3C_2-IONPs-SPs nanocomposites reach to the maximum temperature. T_{max} means the maximum temperature.

$$\eta = \frac{hs(Tmax - Tsurr) - QDis}{I(1 - 10^{-A808})} \quad (6)$$

I is 500 mW, Q_{Dis} is measured independently to be 0.27 mW, and $(T_{max}\text{-}T_{surr})$ is 30.3 °C according to (Fig. 5d). A_{808} is the absorbance (1.58) of Ti_3C_2-IONPs-SPs nanocomposites at 808 nm (Fig. 5e). Now, only hS is unknown for calculating η. We define θ as the following equation.

$$\theta = \frac{T - Tsurr}{Tmax - Tsurr} \quad (7)$$

The sample system time constant τ_s.

$$\tau_s = \frac{\sum_i m_i C_{p,i}}{hs} \quad (8)$$

τ_s is substituted into equation (2) and obtained.

$$\frac{d\theta}{dt} = \frac{1}{\tau s}\left[\frac{Q_{Ti3C2-IONPs-SPs} + Q_{Dis}}{hs(Tmax - Tsurr)} - \theta\right] \quad (9)$$

When the laser was shut off, the temperature of Ti_3C_2-IONPs-SPs cooling down. ($Q_{Ti3C2-IONPs-SPs} + Q_{Dis}$) equals zero, getting the following equation.

$$dt = -\tau_s \frac{d\theta}{\theta} \quad (10)$$

and the equation could be translated into

$$t = -\tau_s \ln\theta \quad (11)$$

According to Fig. S5, time constant for heat transfer of the whole system is determined to be τ_s = 161 s according to the linear time data from the cooling stage *versus* negative natural

logarithm of driving force temperature. In addition, m is 0.3 g and C is 4.2 J g^{-1}. According to equation (8), the hs is calculated as 7.83 mW/°C. Putting this numerical value into equation (6), and the photothermal-convention efficiency (η) of Ti_3C_2-IONPs-SPs nanocomposites can be calculated to be 48.6%.

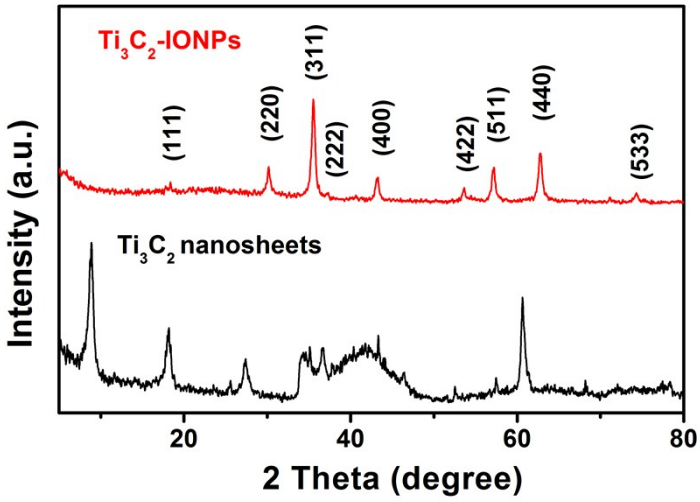

Fig. S1 X-ray diffraction (XRD) profiles of Ti_3C_2 nanosheets and Ti_3C_2-IONPs nanocomposites.

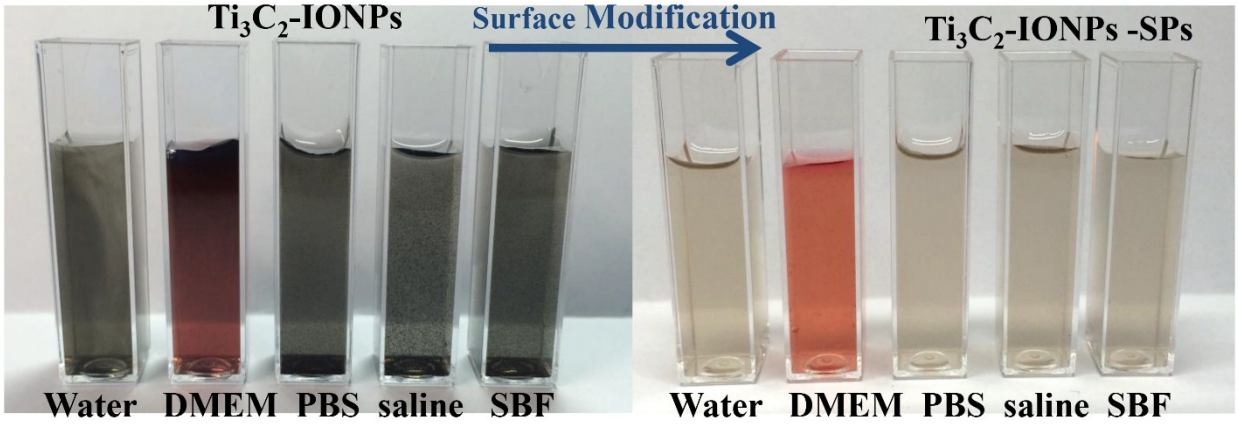

Fig. S2 Photographs of Ti_3C_2-IONPs and Ti_3C_2-IONPs-SPs dispersed in diverse solutions (water, DMEM, PBS, saline and SBF).

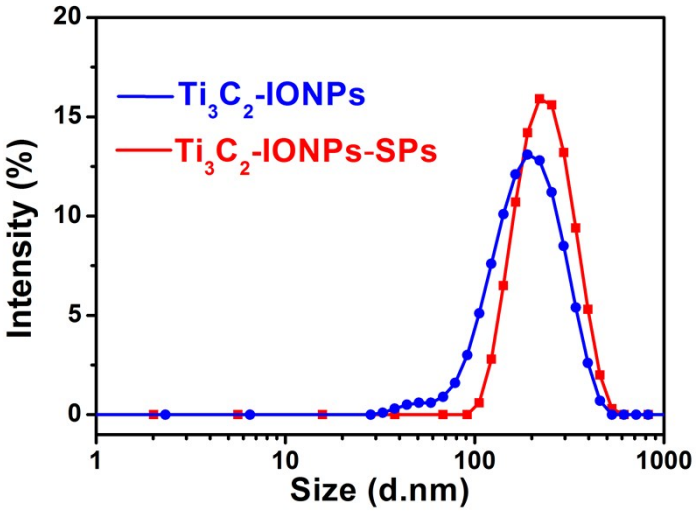

Fig. S3 Dynamic light scattering (DLS) curves of Ti_3C_2-IONPs and Ti_3C_2-IONPs-SPs in aqueous solution.

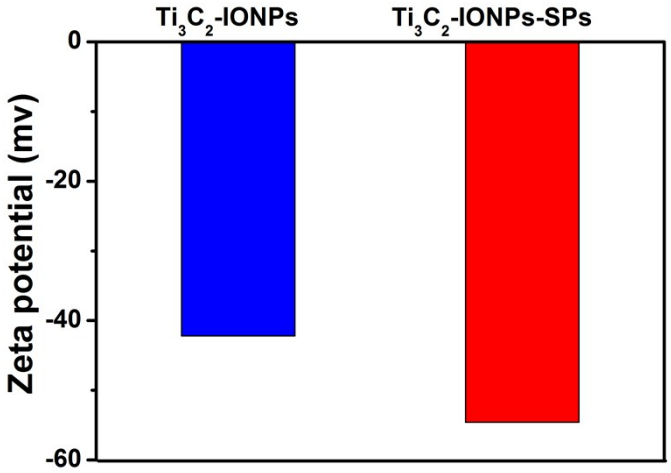

Fig. S4 Zeta potential of Ti_3C_2-IONPs and Ti_3C_2-IONPs-SPs in aqueous solution.

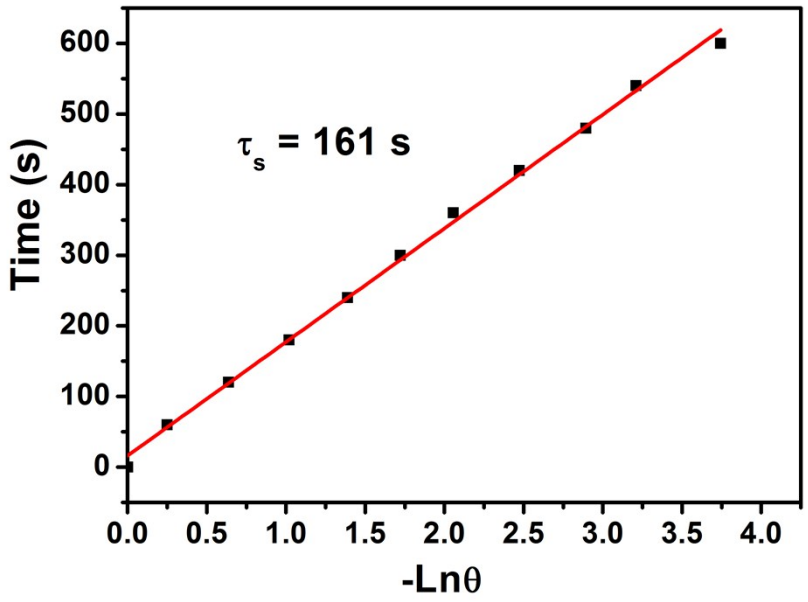

Fig. S5 Time-constant of heat transfer from the system (τ_s = 161 s) by applying the linear time value from the cooling stage (600 s) against negative natural logarithm of driving-force temperature.

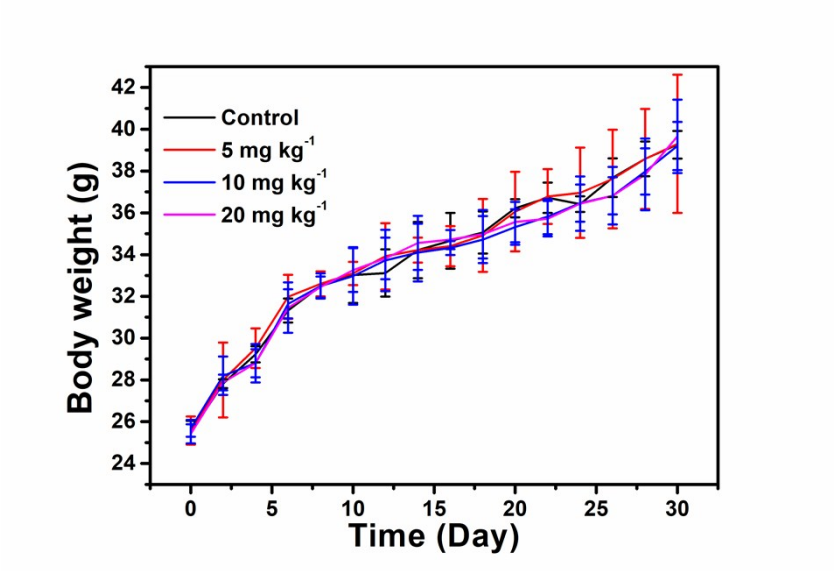

Fig. S6 Time-dependent body-weight changing profiles of Kunming mice within 30 days after intravenous administration of Ti_3C_2-IONPs-SPs at elevated doses (0, 5, 10 and 20 mg kg^{-1}).

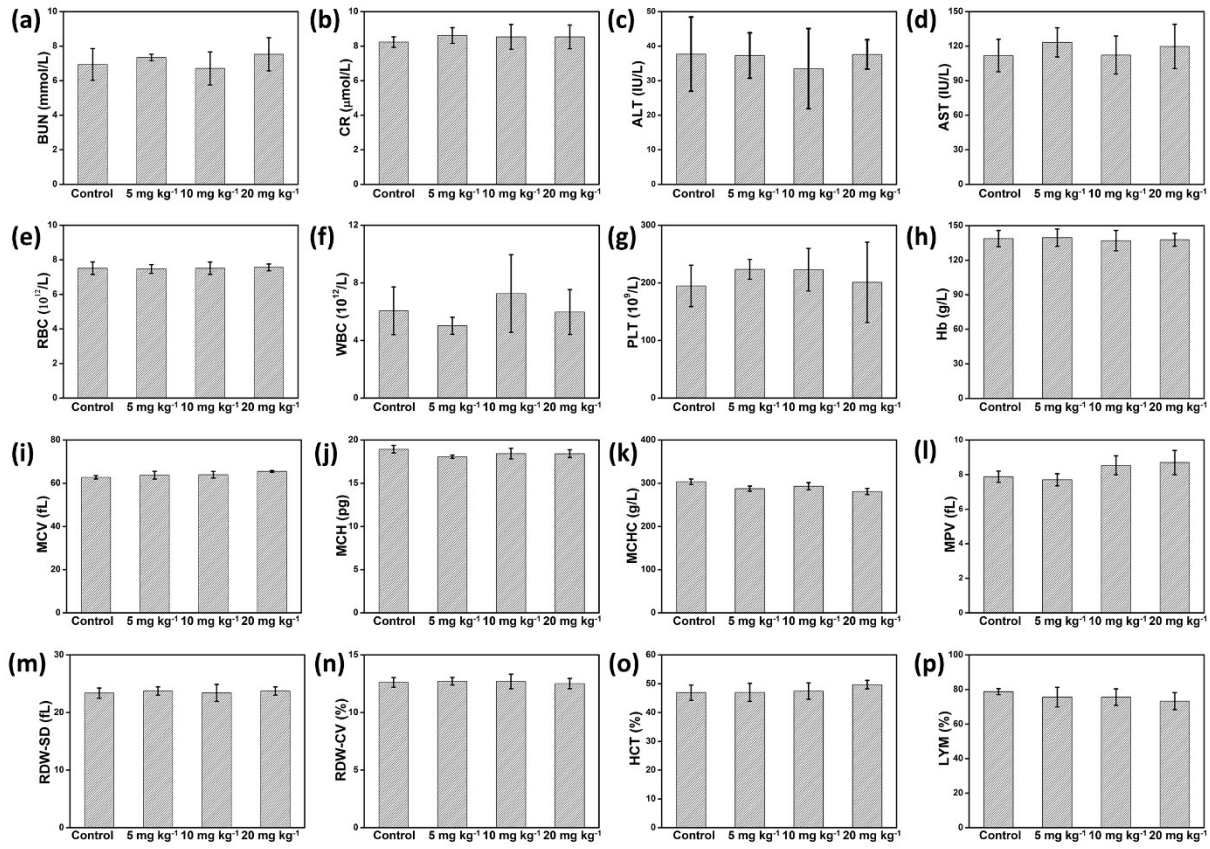

Fig. S7 Hematological test of Kunming mice from the control group and three treatment groups at 30th days after intravenous injection of Ti_3C_2-IONPs-SPs.

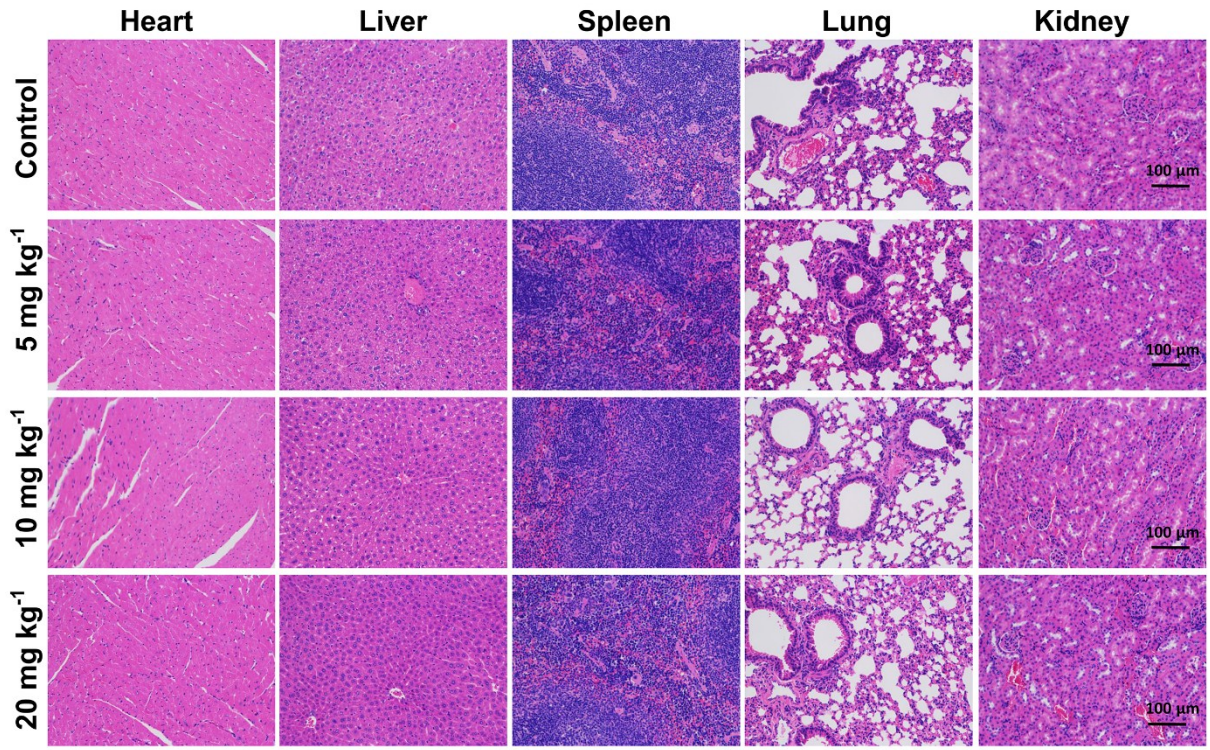

Fig. S8 H&E staining tissue sections of main organs including heart, liver, spleen, lung and kidney of Kunming mice after single intravenous injection of Ti_3C_2-IONPs-SPs at elevated doses (0, 5, 10 and 20 mg kg^{-1}).

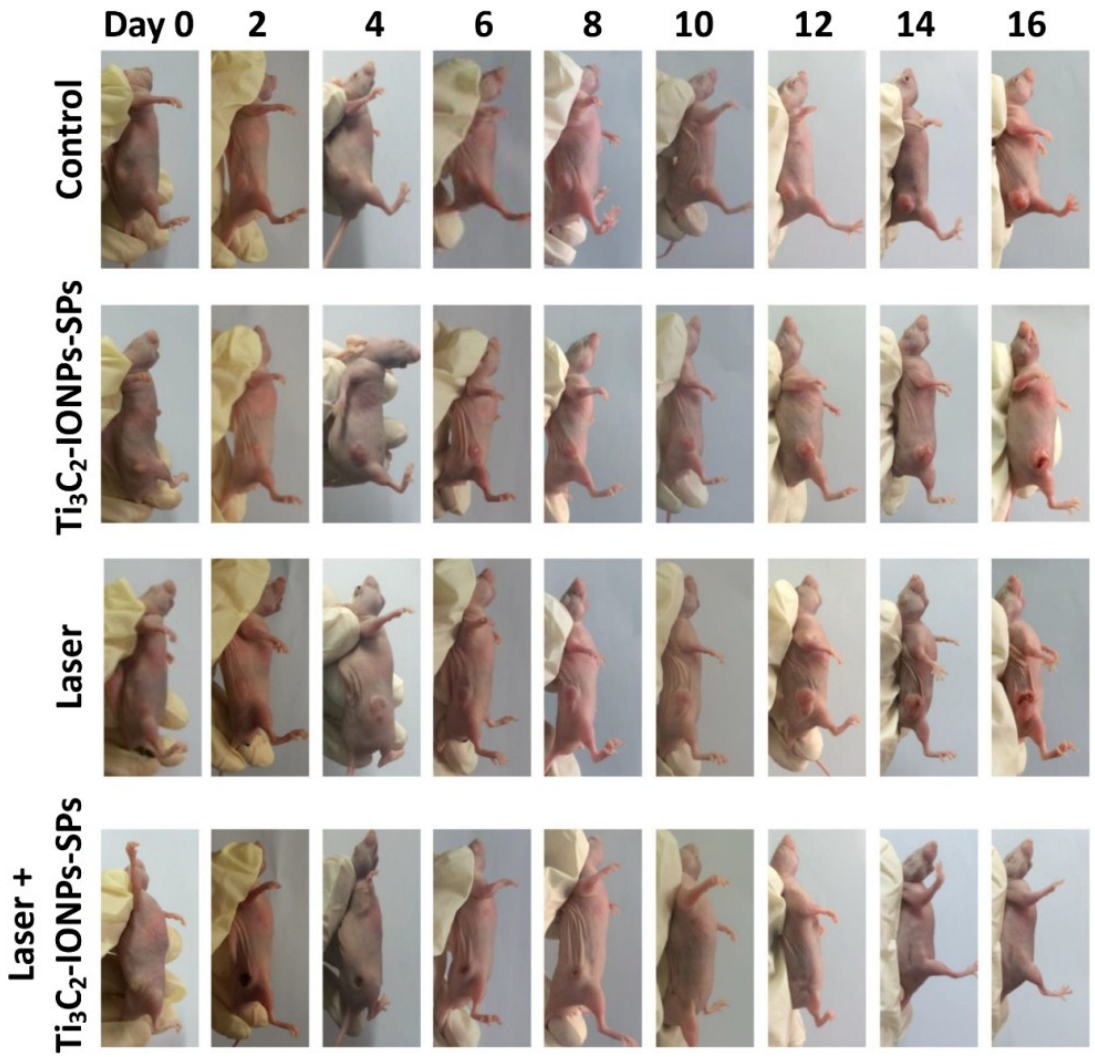

Fig. S9 Digital photography of 4T1 tumor-bearing BALB/c nude mice in different treatment groups as taken within 16 days.

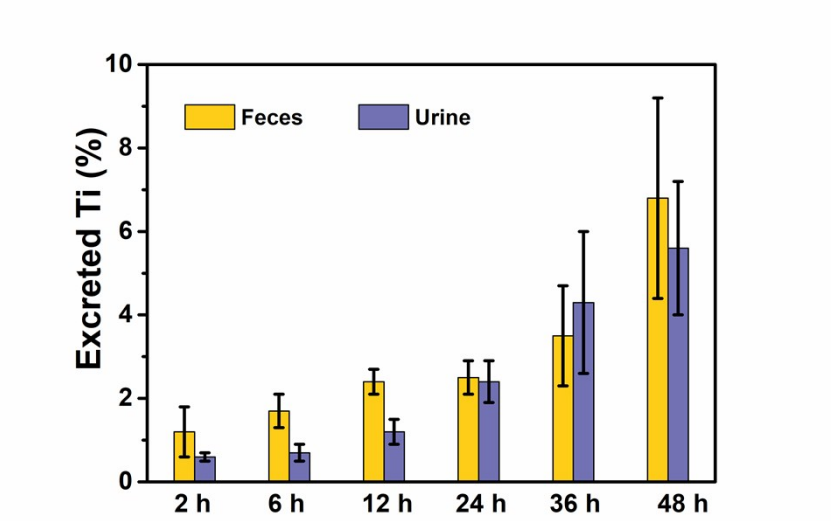

Fig. S10 Accumulated (feces and urine) Ti excretion out of the health Kunming mice after the intravenous administration of Ti_3C_2-IONPs-SPs for different durations.

References.

1 H. Lin, X. Wang, L. Yu, Y. Chen and J. Shi, *Nano lett.*, 2017, **17**, 384-391.
2 D. K. Roper, W. Ahn, M. Hoepfner, *J. Phys. Chem. C*, 2007, **111**, 3636-3641.