

Supporting information for

**Dynamically Tuning Near-infrared-induced Photothermal Performances  
of TiO<sub>2</sub> Nanocrystals by Nb-doping for Imaging Guided Photothermal  
Therapy of Tumors**

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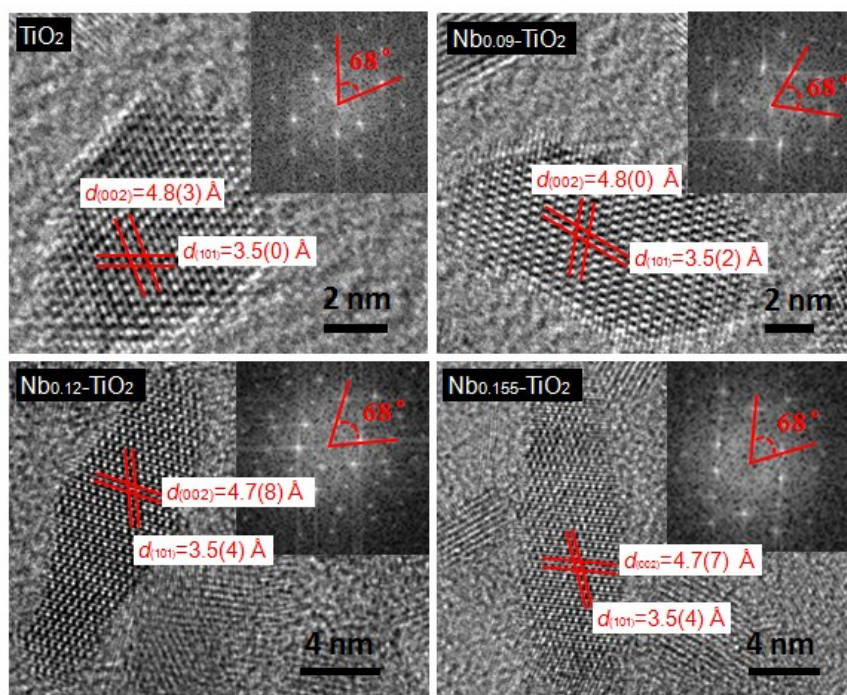
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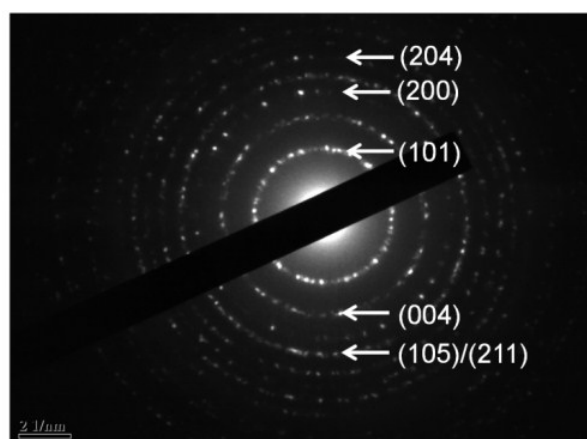
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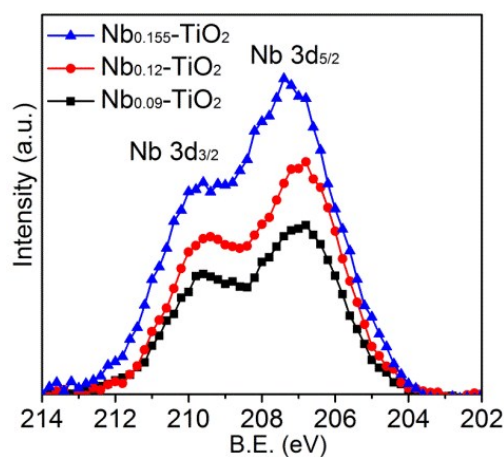
**Fig. S1** HR-TEM images and the corresponding FFT patterns of the pure  $\text{TiO}_2$  and Nb-doped  $\text{TiO}_2$  samples.



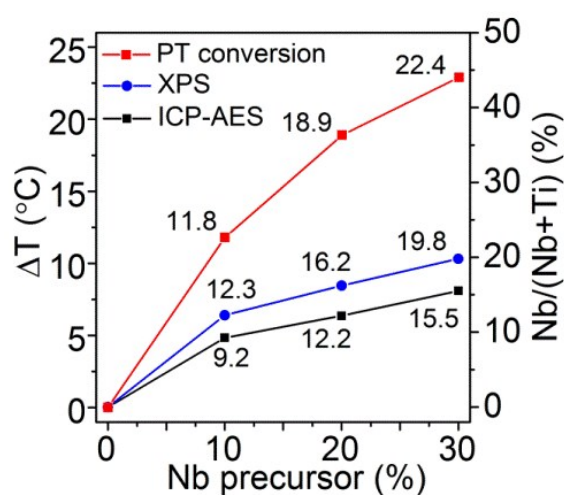
**Fig. S2** SAED pattern of  $\text{Nb}_{0.12}\text{-TiO}_2$  sample.

**Table S1.** The detail peak positions for the fitted peaks.

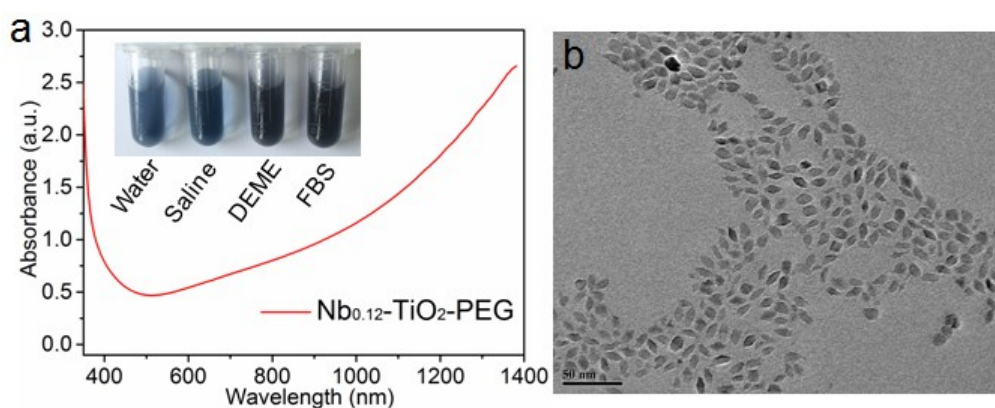
| Samples                          | $\text{Ti}^{4+}$<br>2p3/2 | $\text{Ti}^{4+}$<br>2p1/2 | $E_g$ | $\text{Ti}^{3+}$<br>2p3/2 | $\text{Ti}^{3+}$<br>2p1/2 | $E_g$ | $\text{Nb}^{5+}$<br>3d5/2 | $\text{Nb}^{5+}$<br>3d3/2 | $E_g$ |
|----------------------------------|---------------------------|---------------------------|-------|---------------------------|---------------------------|-------|---------------------------|---------------------------|-------|
| $\text{Nb}_{0.155}\text{-TiO}_2$ | 459.25                    | 464.9                     | 5.65  | 456.9                     | 462.5                     | 5.6   | 207.1                     | 209.9                     | 2.8   |
| $\text{Nb}_{0.12}\text{-TiO}_2$  | 459.2                     | 464.9                     | 5.7   | 456.8                     | 462.4                     | 5.6   | 206.84                    | 209.64                    | 2.8   |
| $\text{Nb}_{0.09}\text{-TiO}_2$  | 459.05                    | 464.7                     | 5.65  | 456.5                     | 462.2                     | 5.7   | 206.85                    | 209.65                    | 2.8   |
| $\text{TiO}_2$                   | 458.6                     | 464.3                     | 5.7   | /                         | /                         | /     | /                         | /                         | /     |



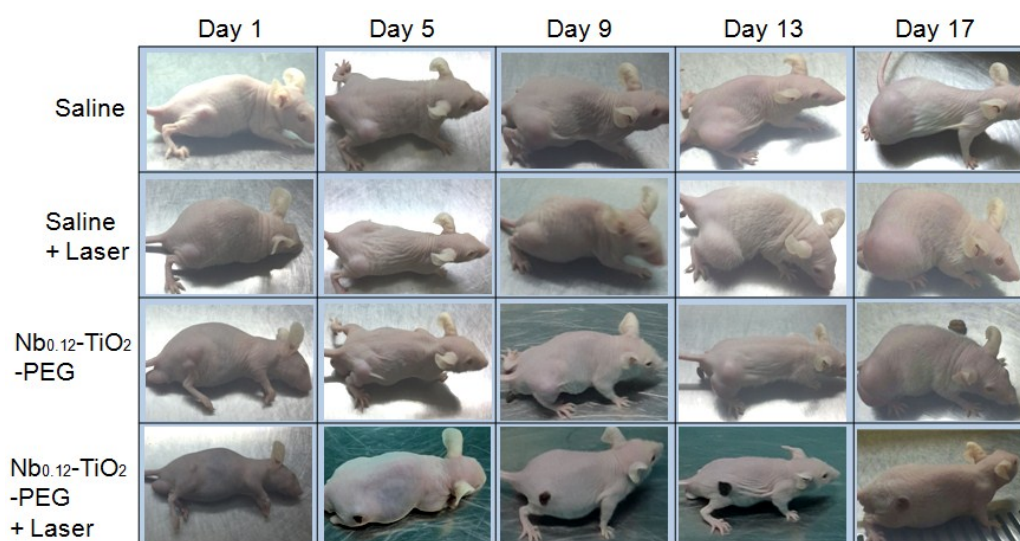
**Fig. S3** Nb 3d spectra of Nb-doped TiO<sub>2</sub> samples.



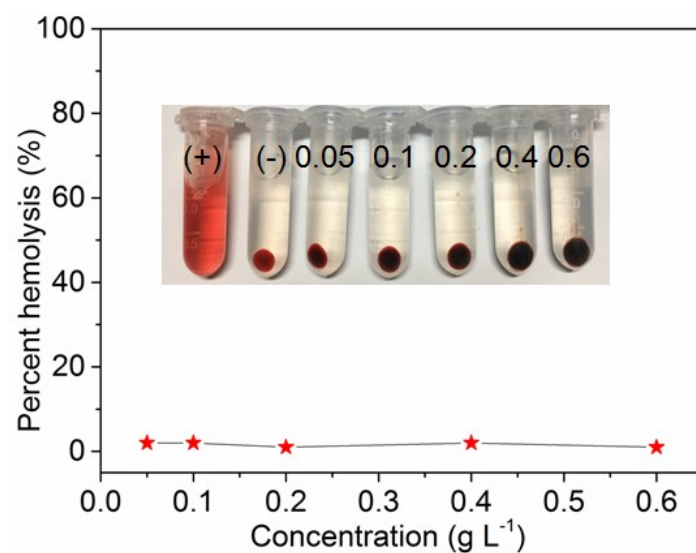
**Fig. S4** The curves of temperature elevation ( $\Delta T$ ) and Nb/(Nb+Ti) atomic ratios (determined by ICP-AES and XPS) of TiO<sub>2</sub> samples as a function of Nb precursor ratios.



**Fig. S5** (a) UV-vis-NIR spectrum of Nb<sub>0.12</sub>-TiO<sub>2</sub>-PEG aqueous dispersion. The inset shows Nb<sub>0.12</sub>-TiO<sub>2</sub>-PEG nanocrystals in different solvent (water, saline, DMEM, FBS) after being stored for one week. (b) TEM image of Nb<sub>0.12</sub>-TiO<sub>2</sub>-PEG.



**Figure S6.** Representative photos of tumors on mouse after treatment with different therapeutic conditions.



**Fig. S7** The hemolytic percent of RBCs incubated with Nb<sub>0.12</sub>-TiO<sub>2</sub>-PEG at various concentrations (0.05, 0.1, 0.2, 0.4, 0.6 g L<sup>-1</sup>) for 4 h, using deionized water (+) and PBS (–) as positive and negative controls, respectively. Inset showing the photograph for direct observation of hemolysis.