

Supporting Information

Near - infrared light - responsive photothermal α -Fe₂O₃@Au/PDA core/shell nanostructure with on-off controllable anti-bacterial effect

Qingshan Xiong^a, Qunling Fang^{a,}, Kezhu Xu^a, Guanghui Liu^c, Min Sang^b, Yunqi Xu^b,
Lingyun Hao^d, Shouhu Xuan^{b,*}*

^a School of Food and Biological Engineering, Key Laboratory of Metabolism and Regulation for Major Diseases of Anhui Higher Education Institutes, Hefei University of Technology, Hefei, 230009, PR China

^b CAS Key Laboratory of Mechanical Behavior and Design of Materials, Department of Modern Mechanics, University of Science and Technology of China, Hefei 230027, PR China

^c School of Energy, Materials and Chemical Engineering, Hefei University, 99 Jinxiu Avenue, Hefei, Anhui, 230601, PR China

^d School of Materials Engineering, Jinling Institute of Technology, Nanjing 211169, PR China

*Corresponding author:

Asso. Prof. Qunling Fang

E-mail: fql.good@hfut.edu.cn

Tel: 86-551-62904353

Fax: 86-551-62904353

Prof. Shouhu Xuan

E-mail: xuansh@ustc.edu.cn

Tel: 86-551-63601702

Fax: 86-551-63606382

1. Synthesis of α -Fe₂O₃@Au/PDA core-shell nanocube.

Firstly, 10 mg α -Fe₂O₃ nanocubes was dispersed in 40 mL EtOH by ultrasonication, then HAuCl₄ (0.15M), trisodium citrate (10 mg) and 30 mL DA-HCl (17.5 mM) in Tris (pH = 8.5) were added to the mixed solution respectively. After sonication for 3 h, the product was obtained from the mixed solution using centrifugal separation and washed 3 times with deionized water and ethanol. At last, the final α -Fe₂O₃@Au/PDA was vacuum dried at 45 °C for 12 h.

2. Preparation of the α -Fe₂O₃@PDA core/shell nanospindle.

10 mg α -Fe₂O₃ was dispersed in 40 mL EtOH by ultrasonication, then 30 mL DA-HCl (17.5 mM) in Tris (pH = 8.5) were added to the mixed solution. After sonication for 6 h, the product was obtained from the mixed solution using centrifugal separation at 8000 rpm and washed 3 times with deionized water and ethanol. Finally, the α -Fe₂O₃@PDA was vacuum dried at 45 °C for 12 h.

3. Fabrication of α -Fe₂O₃@Au/PDA@Au/PDA core-shell nanospindle.

HAuCl₄ (0.15M), trisodium citrate (10 mg) and 30 mL DA-HCl (17.5 mM) in Tris (pH = 8.5) were added to the EtOH (40 mL) dispersed with 10 mg α -Fe₂O₃@Au/PDA nanospindles, after sonication for 3 h, the solid particle was separated from the mixed solution by centrifugal separation at 8000 rpm and washed 3 times with deionized water and ethanol. Finally, the α -Fe₂O₃@Au/PDA@Au/PDA was vacuum dried at 45 °C for 12 h.

4. The photothermal conversion efficiency of the α -Fe₂O₃@Au/PDA core/shell nanostructure

The the scatter in black in Figure. 8d mean time data from the cooling period versus negative natural logarithm of driving force temperature which was obtained from the cooling process. The curve in red was used for calculating the time constants for heat transfer of the α -Fe₂O₃@Au/PDA which were determined to be $\tau_s = 311.69$. The

photothermal conversion efficiency of the α -Fe₂O₃@Au/PDA core/shell nanostructure was calculated according to the reported method.¹ The η value was calculated by the following formula:

$$\eta = \frac{-hS(T_{max} - T_{Surr}) - Q_S}{I(1 - 10^{-A_{808}})} \times 100\%$$

h and S were the heat transfer coefficient and the surface area of the sample container respectively; T_{max} and T_{Surr} were the equilibrium temperature and the ambient temperature of the surroundings; Q_S was expressed as the heat associated with the light absorbance, I was the laser power and A_{808} was the absorbance of the sample at 808 nm.

References

1. W.-N. Wang, C.-Y. Zhang, M.-F. Zhang, P. Pei, W. Zhou, Z.-B. Zha, M. Shao and H.-S. Qian, *Chem. Eng. J.*, 2020, **381**, 125488.

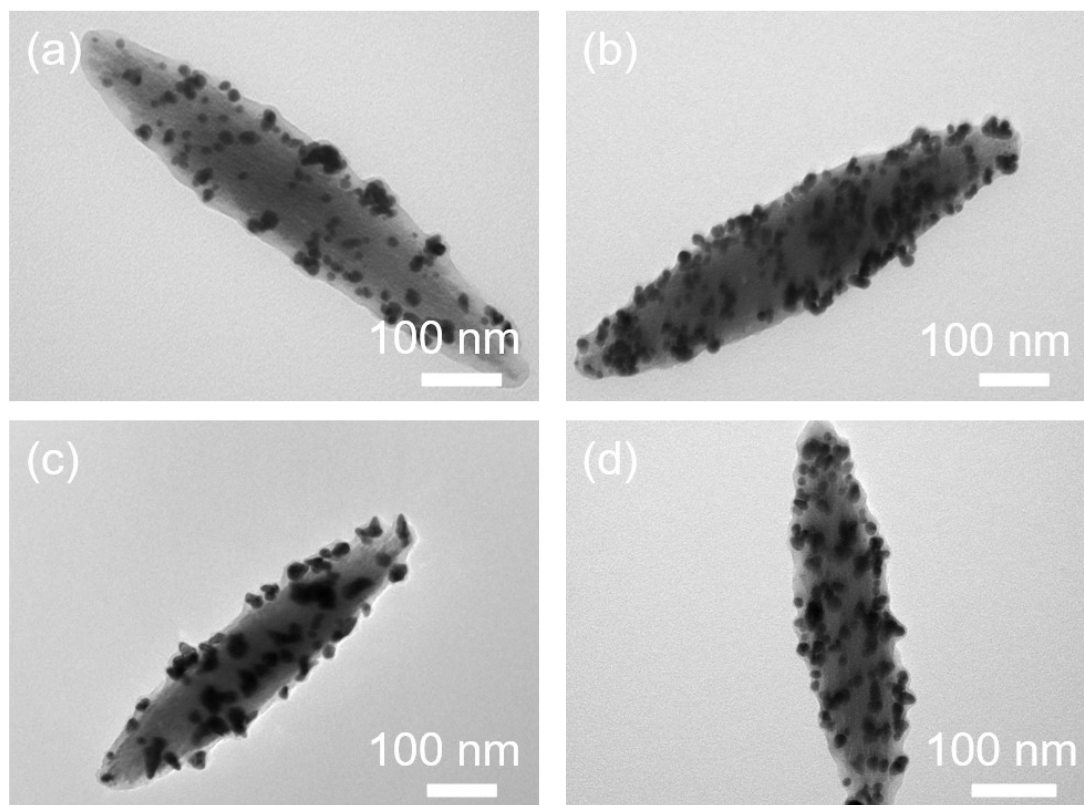


Figure S1. TEM images of α -Fe₂O₃@Au/PDA nanospindle prepared under the same

conditions of DA (30 mg), with different concentrations of H_{AuCl}₄: 4.8×10^{-5} M (a), 7.2×10^{-5} M (b), 9.6×10^{-5} M (c), and 1.2×10^{-4} M (d).

Concentrations of H _{AuCl} ₄ (M)	Au wt%
4.8×10^{-5}	7.8
7.2×10^{-5}	12.0
9.6×10^{-5}	14.3
1.2×10^{-4}	17.6

Table S1. The percent of Au in α -Fe₂O₃@Au@PDA with different concentrations of H_{AuCl}₄.

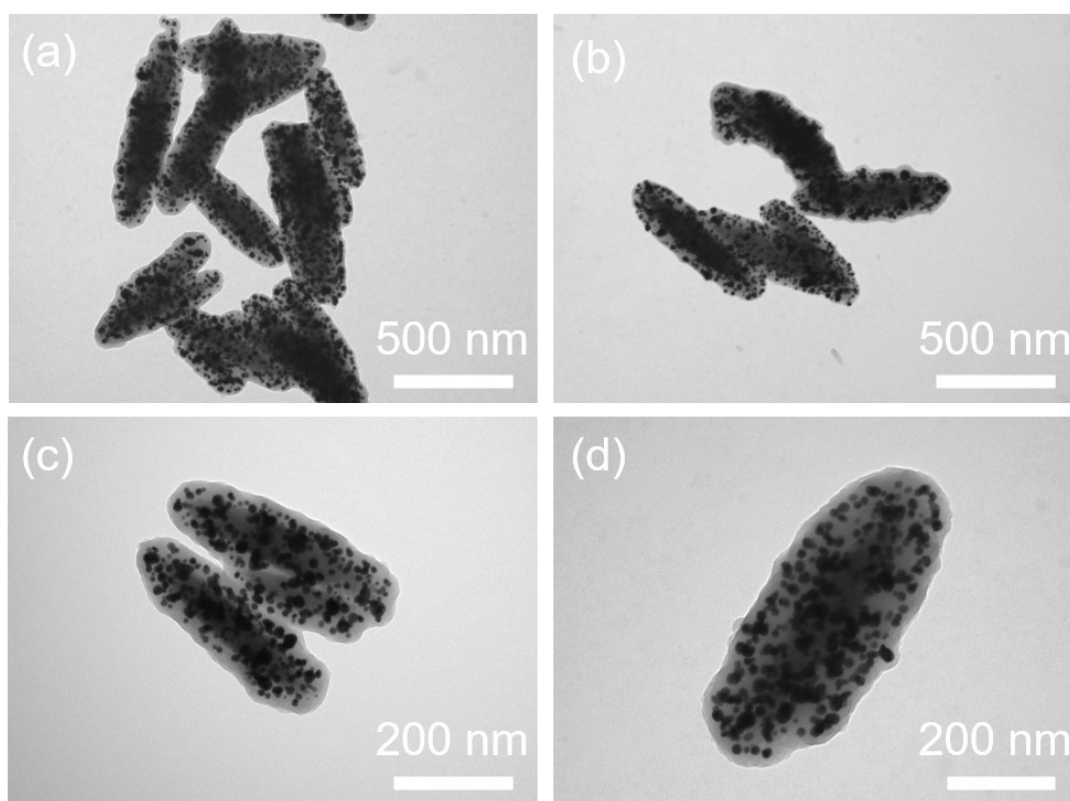


Figure S2. TEM images of spindle α -Fe₂O₃@Au/PDA@Au/PDA prepared with 2.4×10^{-4} M H_{AuCl}₄ and 120 mg PDA.

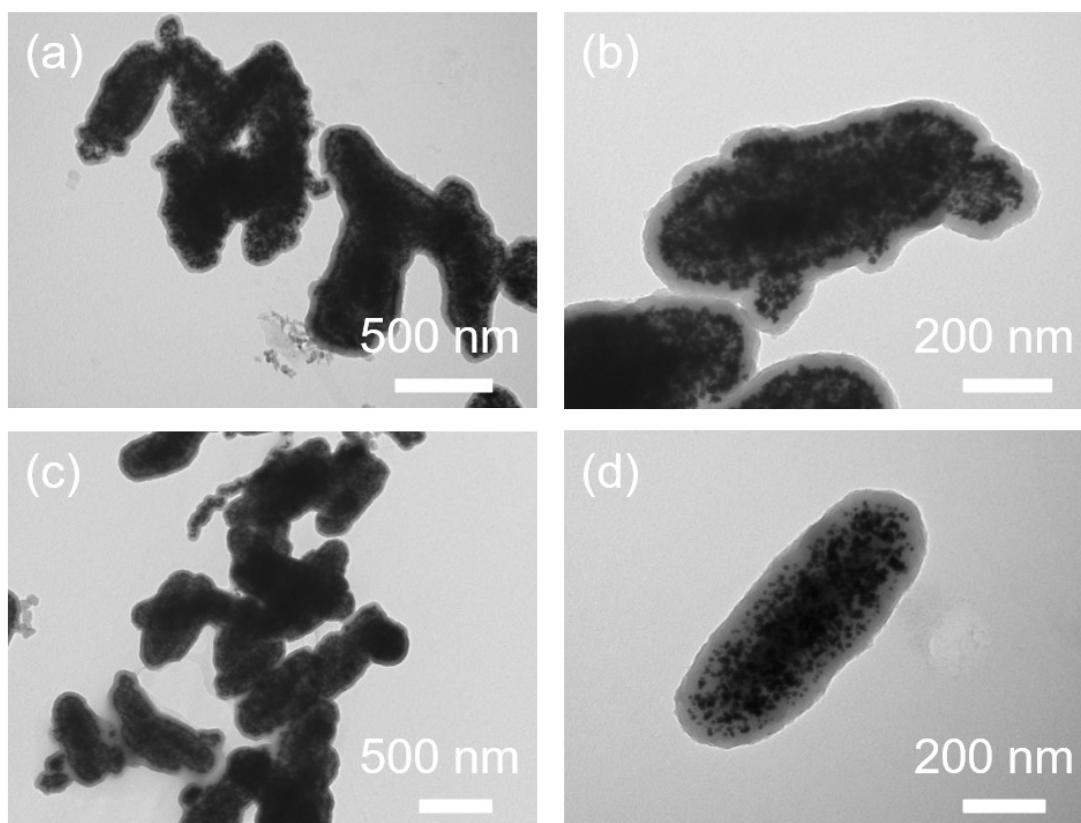


Figure S3. TEM images of spindle $\alpha\text{-Fe}_2\text{O}_3@Au/PDA@Au/PDA@Au/PDA$ prepared with 3.6×10^{-5} M HAuCl_4 and 180 mg PDA.

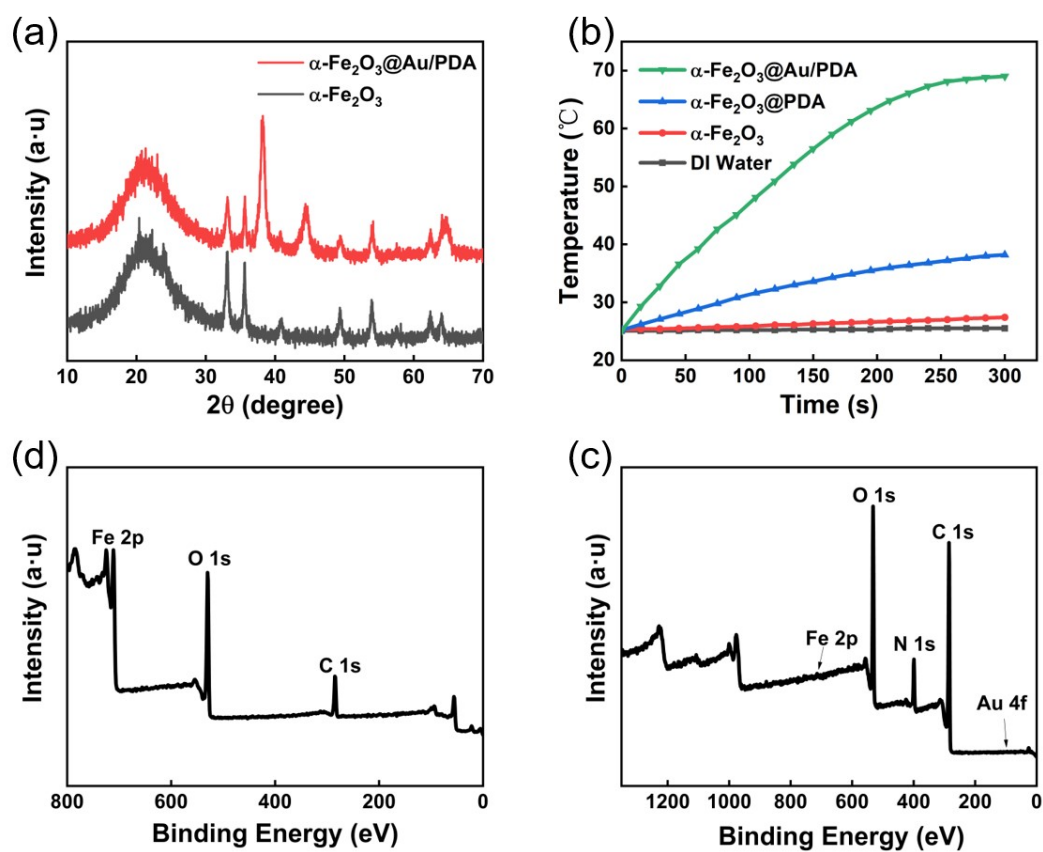


Figure S4. XRD diffraction patterns (a), temperature elevation curves of DI water, cubic $\alpha\text{-Fe}_2\text{O}_3$ (50 $\mu\text{g/mL}$), cubic $\alpha\text{-Fe}_2\text{O}_3\text{@PDA}$ (50 $\mu\text{g/mL}$), cubic $\alpha\text{-Fe}_2\text{O}_3\text{@Au/PDA}$ (50 $\mu\text{g/mL}$), under NIR laser irradiation (808 nm, 2.0 W cm^{-2}) (b), and X-ray photoelectron spectroscopy (XPS) spectra of $\alpha\text{-Fe}_2\text{O}_3$ (c) and $\alpha\text{-Fe}_2\text{O}_3\text{@Au/PDA}$ (d) nanocubes.

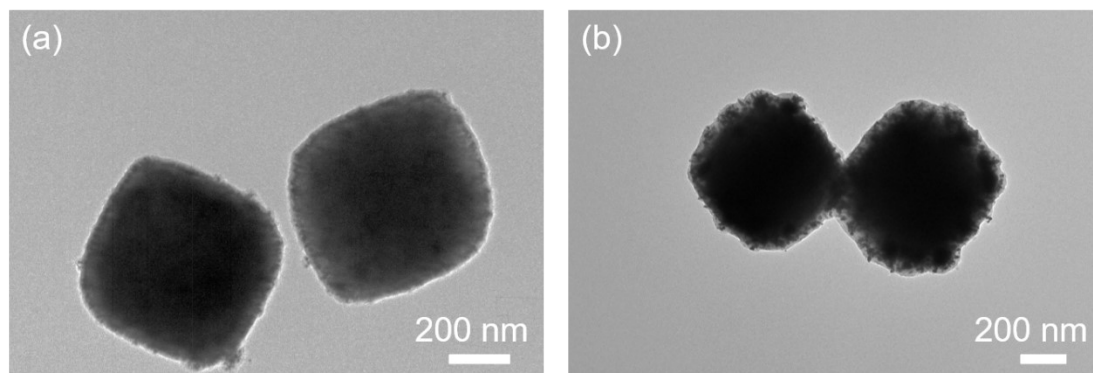


Figure S5. TEM images of cube $\alpha\text{-Fe}_2\text{O}_3\text{@Au/PDA}$ prepared with 7.2×10^{-5} M HAuCl_4 and 60 mg PDA (a), 1.2×10^{-4} M HAuCl_4 and 100 mg PDA (b).

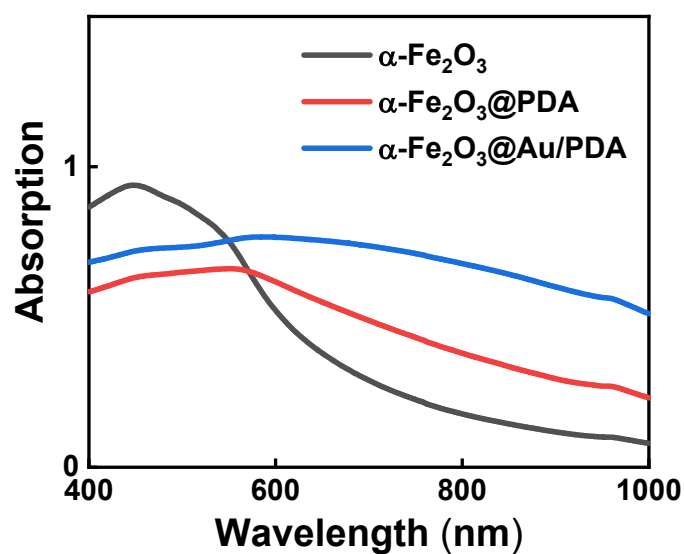


Figure S6. The UV-vis spectra of spindle-like $\alpha\text{-Fe}_2\text{O}_3$, $\alpha\text{-Fe}_2\text{O}_3\text{@PDA}$ and $\alpha\text{-Fe}_2\text{O}_3\text{@Au@PDA}$.

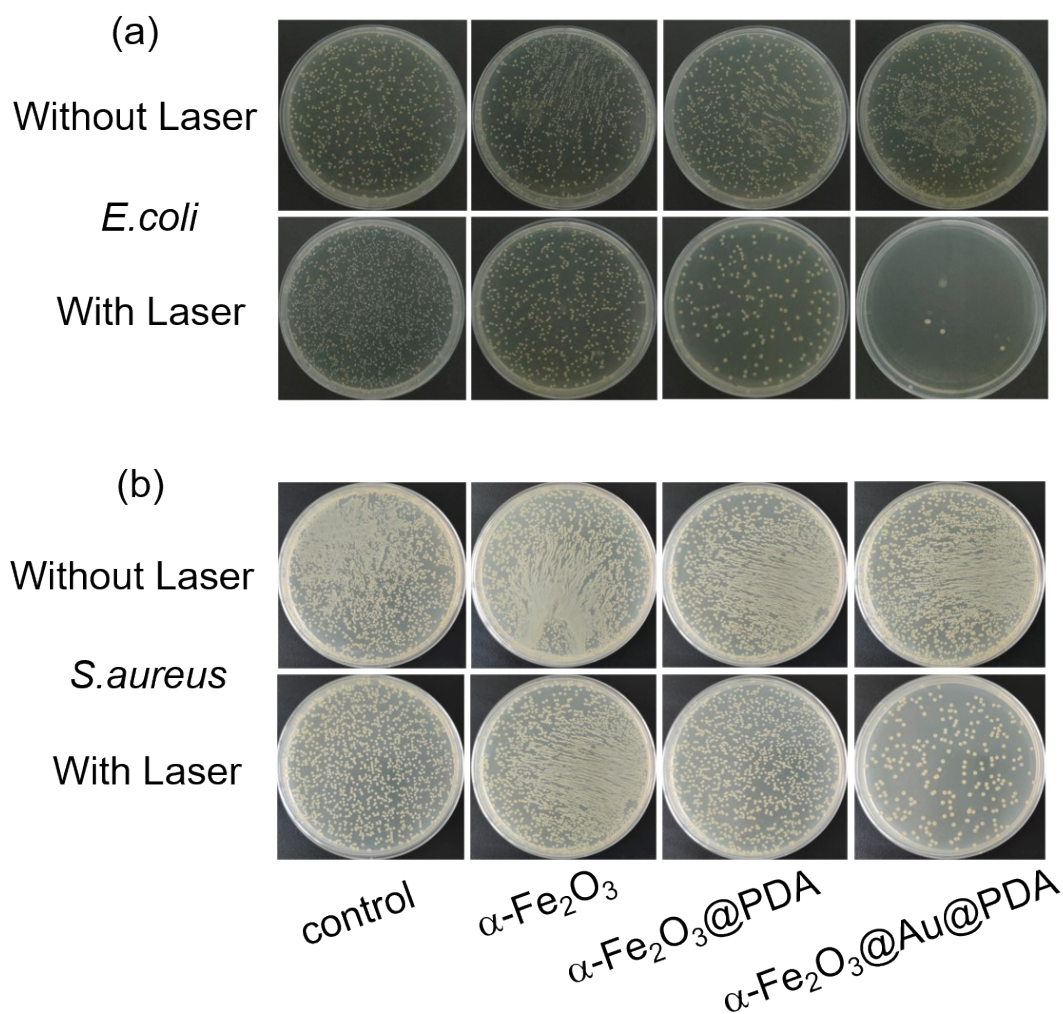


Figure S7. Photographs of colonies of *E. coli* and *S. aureus* incubated with DI water, $\alpha\text{-Fe}_2\text{O}_3$ nanocube, $\alpha\text{-Fe}_2\text{O}_3\text{@PDA}$ nanocube, and $\alpha\text{-Fe}_2\text{O}_3\text{@Au/PDA}$ nanocube (50 $\mu\text{g/mL}$) with/without 808 nm laser irradiation for 5 min.

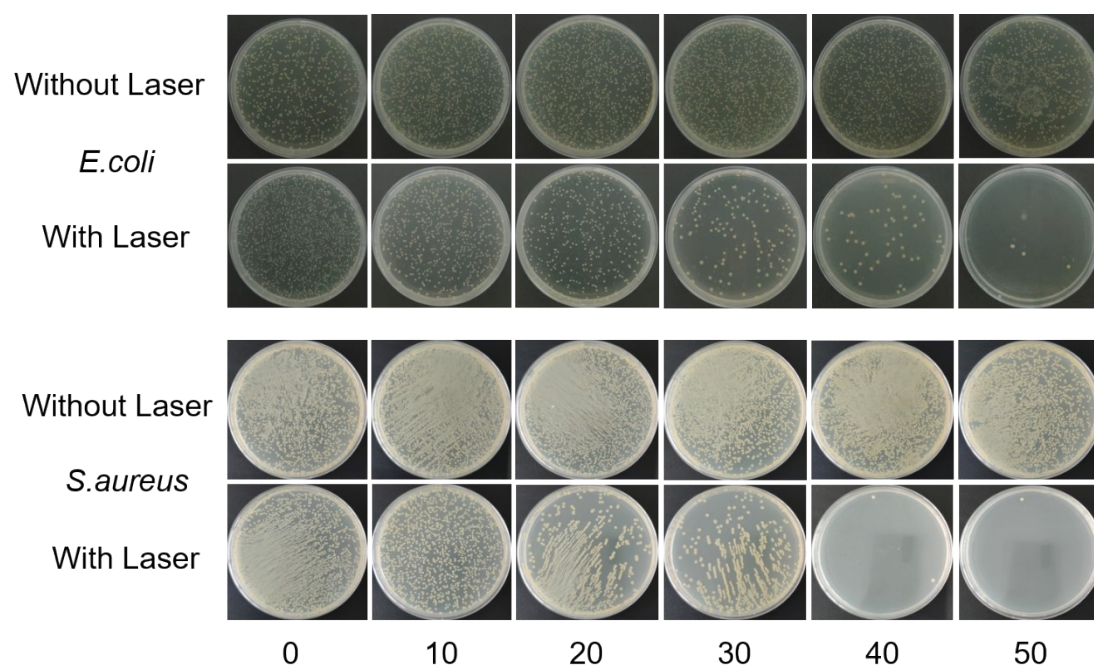


Figure S8. Photographs of colonies of *E. coli* and *S. aureus* incubated with various concentrations (0, 10, 20, 30, 40 and 50 $\mu\text{g/mL}$) of $\alpha\text{-Fe}_2\text{O}_3\text{@Au/PDA}$ nanocubes with/without 808 nm laser irradiation for 5 min.