## pH-Responsive Au@Pd Bimetallic Core-Shell Nanorods for Enhanced Synergistic Targeted Photothermal-Augmented Nanocatalytic Therapy in the Second Near-Infrared Window

Zhe Tang<sup>a#</sup>, Israt Ali<sup>b#</sup>, Yike Hou<sup>a</sup>, Ozioma Udochukwu Akakuru<sup>c</sup>, Quan Zhang<sup>a</sup>, Asim Mushtaq<sup>a</sup>, Han Zhang<sup>a</sup>, Yuguang Lu<sup>a</sup>, Xuehua Ma<sup>d</sup>, Jian Ge<sup>e</sup>, M. Zubair Iqbal<sup>a\*</sup>, Xiangdong Kong<sup>a\*</sup>

<sup>a</sup>Institute of Smart Biomedical Materials, School of Materials Science and Engineering, Zhejiang Sci-Tech University, Hangzhou 310018, China.

<sup>b</sup>Institute National de la Recherche Scientifique, Énergie Matériaux Télécommunications Research Centre 1650 Lionel-Boulet Blvd.Varennes, Quebec J3X 1P7, Canada

<sup>c</sup>Department of Chemical and Petroleum Engineering, Schulich School of Engineering, University of Calgary, Alberta, Canada

<sup>d</sup>Cixi Institute of Biomedical Engineering, CAS Key Laboratory of Magnetic Materials and Devices, Key Laboratory of Additive Manufacturing Materials of Zhejiang Province, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, 1219 Zhongguan West Road, Ningbo, Zhejiang, 315201, China

<sup>c</sup>College of Life Sciences, China Jiliang University, 258 XueYuan Street, XiaSha Higher Education Zone, Hangzhou, 310018, Zhejiang Province, China

Corresponding authors email: kongxd@zstu.edu.cn, zubair@zstu.edu.cn



Fig. S1. EDS spectrum of Au@Pd HNRs.



Fig. S2 Average hydrodynamic dimensions of AuNRs and Au@PdNRs during long-

term storage



**Fig. S3**. FTIR spectra of the Au@Pd-CS, FA, FITC, Au@Pd-CS-FA, and Au@Pd-CS-FA-FITC



Fig. S4. Au NRs and Au@Pd of the same Au-based concentrations (18.75  $\mu$ g mL<sup>-1</sup>)., a single cycle diagram irradiated by 1064 nm (1.0 W cm<sup>-2</sup>) laser for five minutes.



Fig. S5. Time-dependent absorbance at 652 nm of TMB $-H_2O_2$  reaction system catalyzed by Au@Pd.



Fig. S6. The image of with or without Au@Pd-CS-FA in H<sub>2</sub>O<sub>2</sub>. Parameters: [H<sub>2</sub>O<sub>2</sub>]:
3%, [Au@Pd-CS-FA]: 40 μg mL<sup>-1</sup>, [Temperature]: 37 °C, [Time]: 20 min.



**Fig. S7.** L929 and 4T1 cells viability incubated with Au@Pd-CS or Au@Pd-CS-FA for 24 h at different concentrations.



Fig. S8. CLSM images of 4T1 cells stained by DCFH-DA to indicate nanoparticle-induced ROS generation. Scale bar:  $25 \ \mu m$ 



**Fig. S9.** H&E staining images of major organs (heart, liver, spleen, lung, and kidney) of healthy nude mice 3 weeks after the tail vein were in vivo injected intravenously with PBS, Au@Pd-CS, and Au@Pd-CS-FA, respectively. Scale bar: 200 μm.



Fig. S10 Biodistribution of Au@Pd-CS-FA HNRs in different organs of 4T1 tumor-



## bearing nude mice at different time points

**Fig. S11** (a) Photothermal images, (b) temperature changes and (c) HNRs content of tumors injected with Au@Pd-CS-FA at different times (12 hours, 24 hours and 36 hours).



**Fig. S12.** (a) Schematic illustration of tumor treatment in vivo (b) representative digital images of the mice under different treatments on different days