Supporting Information

Regulating Thermal Diffusion of Gold Thin Film at Solid-State Interfaces for Site-Selective Decoration of Gold Nanoparticles on Titania Nanotubes as Efficient SERS Sensing Platform

Zhiyan Hu, Shan Chen, Yue Shi, Fengyu Yuan, Fengjiao Yu, Jun Fang and Yang Yang*

State Key Laboratory of Materials-Oriented Chemical Engineering, College of Chemical Engineering, Nanjing Tech University, Nanjing 211816, China

*Corresponding Author; email: yangy@njtech.edu.cn

Figures



Figure S1. (a) SEM and (b) TEM images of ZnO-Au-TiO₂ annealed at 500 °C.



Figure S2. Integrated EDX spectrum of Au-TiO₂.



Figure S3. X–Y view of the FDTD simulation models used for the calculation of the EM field enhancement. A 532-nm sinusoidal plane electromagnetic wave and a periodic boundary condition were used in the simulations. The Au dielectric constant used is from Johnson and Christy, and the constant for TiO₂ is from Palik.



Figure S4. (a–c) X–Y view of the FDTD simulation models of Au-TiO₂, TiO₂-Au, and TiO₂-Au-TiO₂ composite nanotubes used for the calculation of the EM field enhancement, where a 20% size distribution of Au nanoparticles is applied. (d–f) FDTD simulations for the EM field enhancement obtained by excitation at 532 nm.



Figure S5. (a–c) X–Y view of the FDTD simulation models of Au-TiO₂, TiO₂-Au, and TiO₂-Au-TiO₂ composite nanotubes used for the calculation of the EM field enhancement in the circumstance of identical Au nanoparticle size and interspace. (d–f) FDTD simulations for the EM field enhancement obtained by excitation at 532 nm.



Figure S6. SERS spectra of R6G molecules obtained from the fresh Au-TiO₂ substrate and the substrate stored in DI water for 10 days.

Calculation details of the analytical enhancement factor

In light of the intricate surface morphology of Au-TiO₂, we employed the following equation to compute the analytical enhancement factor (AEF).

$$AEF = \frac{I_{\text{SERS}} \times C_{\text{R}}}{I_{\text{R}} \times C_{\text{SERS}}}$$

 I_{SERS} and I_{R} represent the Raman intensities of the R6G SERS spectra peak at 612 cm⁻¹, which were acquired from the Au-TiO₂ substrate and the Si wafer substrate, respectively. Meanwhile, C_{SERS} and C_{R} denote the R6G concentrations used for the SERS-active substrate and the Si wafer substrate. In this investigation, I_{SERS} and C_{SERS} were measured at 287 and 10⁻⁹ M, respectively, while I_{R} and C_{R} were recorded as 432 and 0.01 M, correspondingly. As a result, the calculated AEF is 6.64×10^6 .