Electronic Supplementary Information (ESI)

Flexible porous silica aerogel decorated with silver nanoparticles as an effective SERS substrate for label-free trace explosives detection

Wei Liu,a,b Zihao Song,a Yifan Zhao,a Yu Liu,b,c Xuan He,b,c* & Sheng Cui a,c*

a College of Materials Science and Engineering, Nanjing Tech University, Nanjing 211800, China;
b Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, China;
c Jiangsu Collaborative Innovation Center for Advanced Inorganic Function Composites, Nanjing 211800, China.
Figure S1 SEM of SiO₂-Ag hybrids at sputtering durations of 90 s (a, b, c), 180 s (d, e, f), 270 s (g, h, i), 360 s (j, k, l), 450 s (m, n, o), 540 s (p, q, r).
Figure. S2 High-resolution TEM image of as-prepared SiO$_2$-Ag hybrids

**XRD experiments**

Figure. S3 XRD patterns of SiO$_2$ aerogel (the red line) and SiO$_2$-Ag hybrids (the black line).

**Optical absorption spectrum**

Figure. S4 the optical absorption spectrum of SiO$_2$-Ag hybrids and SiO$_2$ aerogel.
**SERS experiments**

![Figure S5](image)

**Figure. S5** Raman responses of SiO$_2$-Ag hybrids in the presence of 4-ATP at different concentrations

![Figure S6](image)

**Figure. S6** Raman responses of 2 μL of 1×10$^{-1}$ M 4-ATP ethanol solution dispersed to an area of 12.25 mm$^2$ for the silicon wafer.

**Text S1.** Detailed calculative process of the enhancement factor

We use the peak at 1439 cm$^{-1}$ (for 4-ATP) to estimate the enhancement factor (EF). The SERS EF is a quantitative measure of the Raman signal amplification of an analyte. The EF can be calculated according to the equation $\text{EF} = (I_{\text{SERS}}/I_{\text{bulk}})(N_{\text{bulk}}/N_{\text{surface}})$. Where $I_{\text{SERS}}$ and $I_{\text{bulk}}$ were the peak intensities of 1×10$^{-10}$ M 4-ATP on SiO$_2$-Ag hybrids and 1×10$^{-1}$ M 4-ATP on the silicon wafer at 1439 cm$^{-1}$, respectively. $N_{\text{surface}}$ and $N_{\text{bulk}}$ are the number of 4-ATP molecules excited by the laser beam on the SiO$_2$-Ag hybrids substrate and the silicon wafer, respectively. Herein, a certain volume ($V_{\text{SERS}}$) and concentration ($C_{\text{SERS}}$) 4-ATP ethanol solution was dispersed to an area of Raman
concentration for non-SERS Raman spectra certain $S_{\text{SERS}}$ at the SiO$_2$-Ag hybrids substrate. For non-SERS Raman spectra, a certain volume ($V_{\text{bulk}}$) and concentration ($C_{\text{bulk}}$) 4-ATP ethanol solution was dispersed to an area of $S_{\text{bulk}}$ at a clean Si substrate. Both the substrates are dried in the air. Considering the area of laser spot is the same, the equation thus becomes: $EF = (I_{\text{SERS}}/I_{\text{bulk}})(C_{\text{bulk}}V_{\text{bulk}}/C_{\text{SERS}}V_{\text{SERS}})(S_{\text{SERS}}/S_{\text{bulk}})$. In our experiment, 2 mL of $1 \times 10^{-9}$ M 4-ATP solution was dispersed to an area of 14 mm$^2$ for the SiO$_2$-Ag hybrids substrate shown in Figure. S4 and 2 μL of $1 \times 10^{-1}$ M 4-ATP ethanol solution is dispersed to an area of 12.25 mm$^2$ for the silicon wafer shown in Figure. S5. For the band at 1439 cm$^{-1}$, $I_{\text{SERS}}/I_{\text{bulk}}$ is $2038/187=10.9$. Therefore average enhancement factor for the band at 1439 cm$^{-1}$ was calculated to be $1.25 \times 10^6$.

**Scheme S1** Samples preparation methods: (a) Dripping the NTO ethanol solution (2 μL) on the surface of the substrates. (b) Soaking the SiO$_2$-Ag hybrids substrate in $1 \times 10^{-5}$ M NTO ethanol solution (2 mL).
**Figure. S7** Raman responses of SiO$_2$-Ag hybrids in the presence of NTO at different concentrations

**Text S2.** Detailed calculative process of the LOD

The standard curve of NTO was plotted as:

$$Y = A + B \times \log_{10} X$$

where, A and B are the variable obtained via least-square root linear regression for the signal-concentration curve and variable Y represents the normalized SERS signal ($I_{\text{NTO}}/I_{\text{blank}}$) at NTO concentration of $X(C_{\text{NTO}})$. where, SD is the standard deviation and $Y_{\text{blank}}$ is the SERS signal of blank sample.

The LOD was calculated as $\text{LOD}=10^\left[\frac{Y_{\text{blank}} + 3\text{SD}}{Y_{\text{blank}} - A}/B\right]$.

SD was calculated according to the well-known formula:

$$\text{SD} = \sqrt{\frac{1}{n-1} \times \sum_{i=1}^{n} (X_i - X_{\text{average}})^2}$$

where, n is the total number of the NTO standard sample. $X_i$ is the “i” sample of the series of measurements. $X_{\text{average}}$ is the average value of the SERS signals obtained for the specific series of identical samples repeated n times.

As shown in Figure. 5(b) and Figure. S6, SD=0.9892, A=6.905, B=-0.530, $Y_{\text{blank}}$=37, The LOD was calculated to be $7.94 \times 10^{-10}$ M.

**Table S1.** The SERS intensity of the 847 cm$^{-1}$ bands from thirty dots.

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