Electronic Supplementary Material (ESI) for Analytical Methods.
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Electronic Supplementary Information (ESI)

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

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SEM measurements

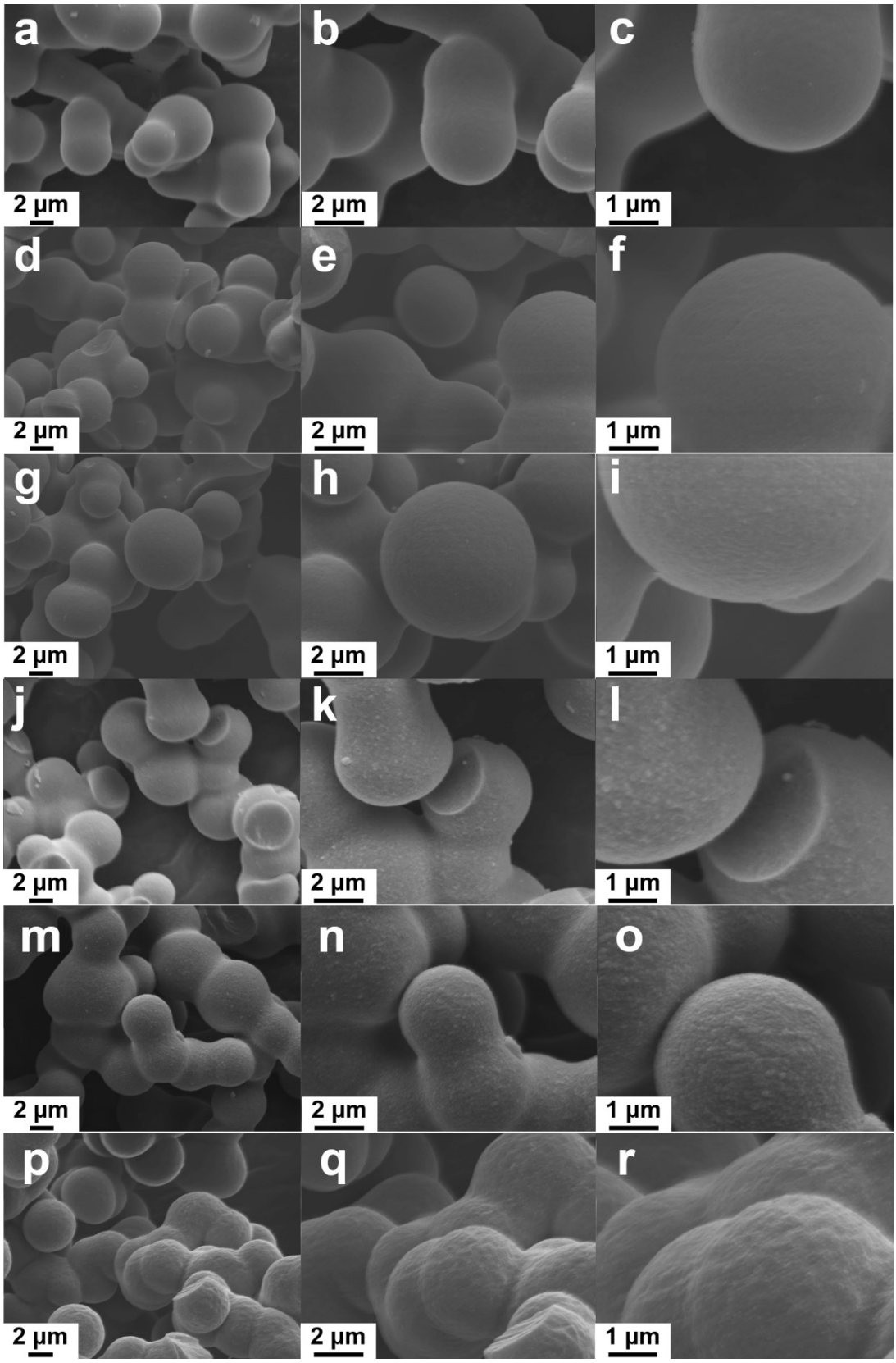


Figure. S1 SEM of SiO_2-Ag hybrids at sputtering durations of 90 s (a, b, c), 180 s (d, e, f), 270 s (g, h, i), 360 s (j, k, l), 450 s (m, n, o), 540 s (p, q, r).

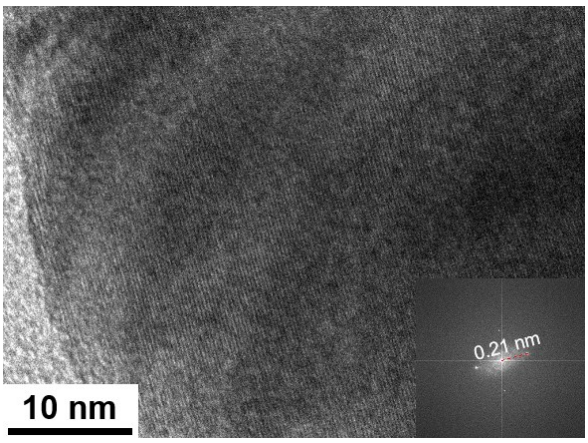


Figure. S2 High-resolution TEM image of as- prepared SiO_2-Ag hybrids

XRD experiments

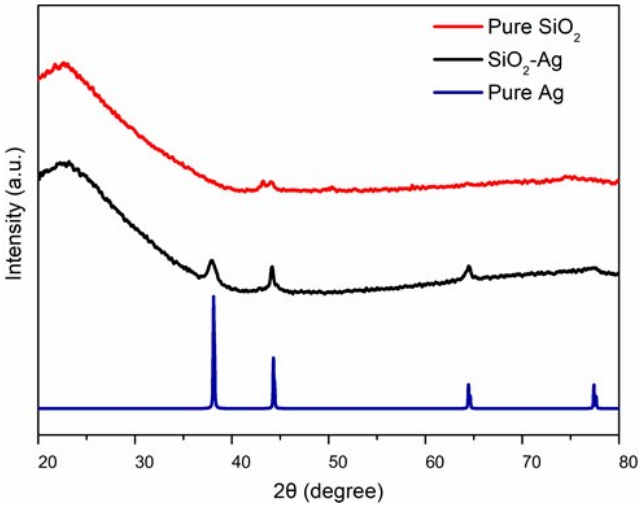


Figure. S3 XRD patterns of SiO_2 aerogel (the red line) and SiO_2-Ag hybrids (the black line).

Optical absorption spectrum

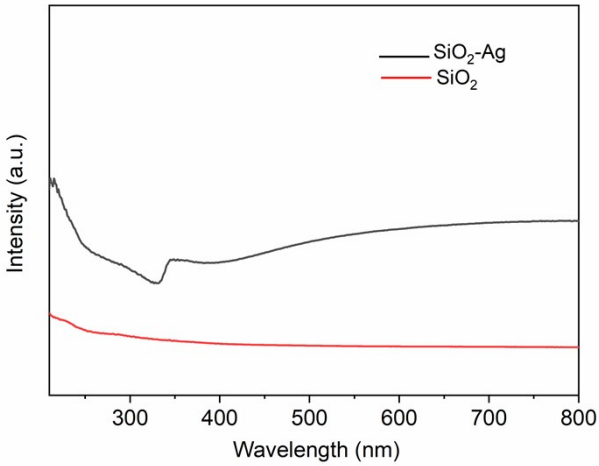


Figure. S4 the optical absorption spectrum of SiO_2-Ag hybrids and SiO_2 aerogel.

SERS experiments

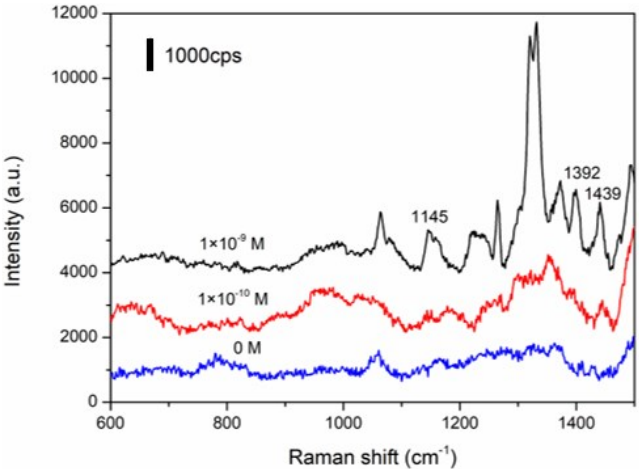


Figure. S5 Raman responses of SiO_2-Ag hybrids in the presence of 4-ATP at different concentrations

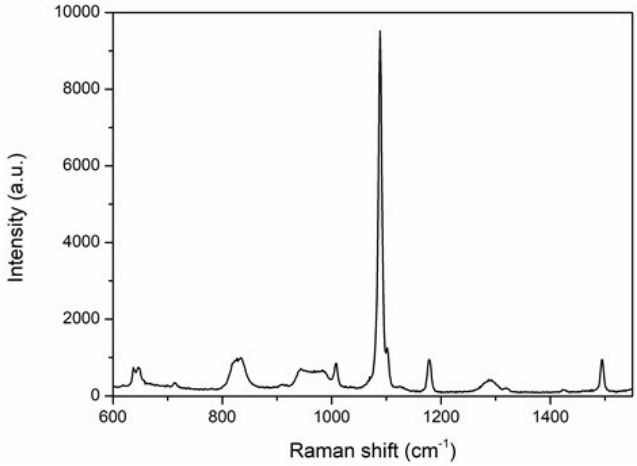
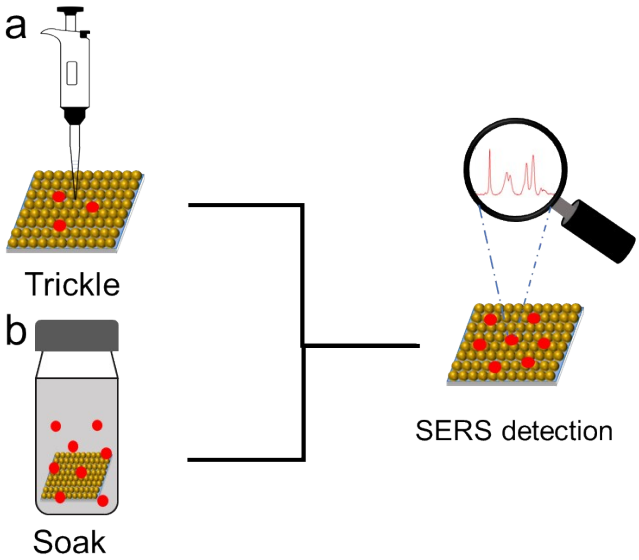


Figure. S6 Raman responses of 2 μL of 1×10^{-1} M 4-ATP ethanol solution dispersed to an area of 12.25 mm^2 for the silicon wafer.

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 EF = $(I_{SERS}/I_{bulk})(N_{bulk}/N_{surface})$. Where I_{SERS} and I_{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. $N_{surface}$ and N_{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_{SERS}) and concentration (C_{SERS}) 4-ATP ethanol solution was dispersed to an area of Raman

concentration for non-SERS Raman spectra certain S_{SERS} at the SiO_2-Ag hybrids substrate. For non-SERS Raman spectra, a certain volume(V_{bulk}) and concentration (C_{bulk}) 4-ATP ethanol solution was dispersed to an area of S_{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: $EF = (I_{SERS}/I_{bulk})(C_{bulk}V_{bulk}/C_{SERS}V_{SERS})(S_{SERS}/S_{bulk})$. In our experiment, 2 mL of 1×10^{-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 1×10^{-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_{SERS}/I_{bulk} is 2038/187=10.9. Therefore average enhancement factor for the band at 1439 cm^{-1} was calculated to be 1.25×10^6.



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 1×10^{-5} M NTO ethanol solution (2 mL).

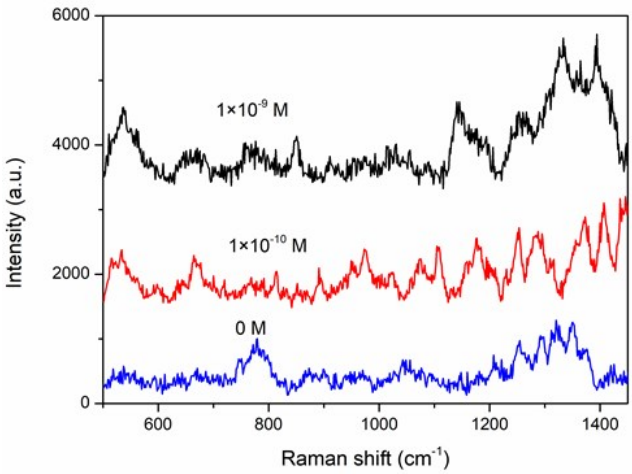


Figure. S7 Raman responses of SiO_2-Ag hybrids in the presence of NTO at different concentrations

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_{NTO}/I_{blank}) at NTO concentration of X(C_{NTO}). where, SD is the standard deviation and Y_{blank} is the SERS signal of blank sample.

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

SD was calculated according to the well-known formula:

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

where, n is the total number of the NTO standard sample. X_i is the "i" sample of the series of measurements. $X_{average}$ 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_{blank}=37, The LOD was calculated to be 7.94×10^{-10} M.

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

Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**

Intensity	23416	25396	24234	21838	25783	22797	21232	26009	20417	21543
Number	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Intensity	22940	23137	22972	21001	23250	22718	23598	21623	2332	22493
Number	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
Intensity	25131	26038	24731	23799	22094	26698	21695	24330	23363	26840