

Supplementary Information

Explosives vapor/particles detection using SERS substrates and hand-held Raman detector

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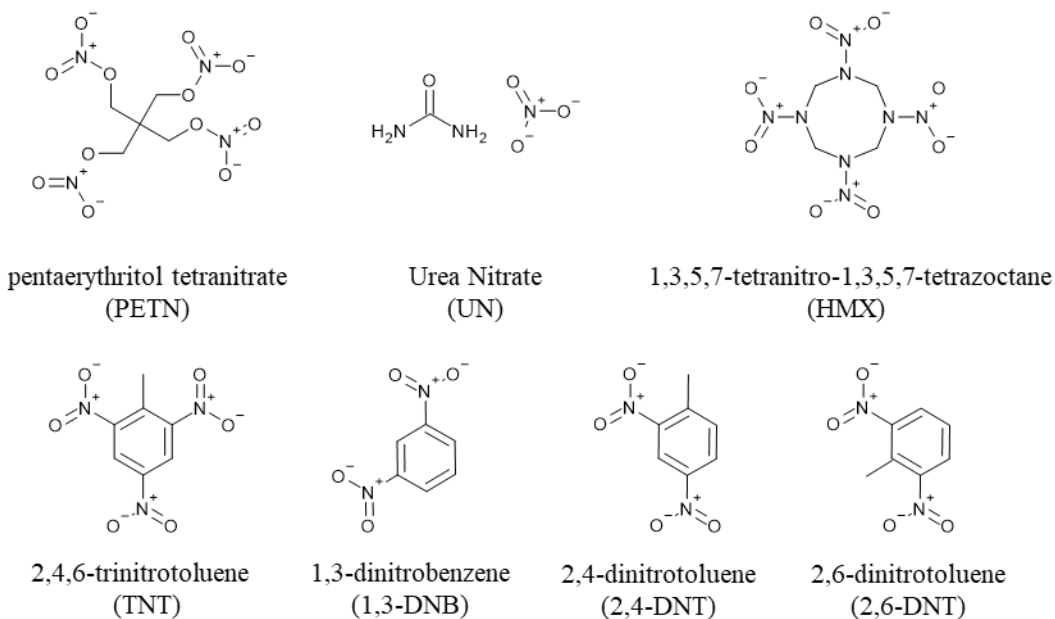
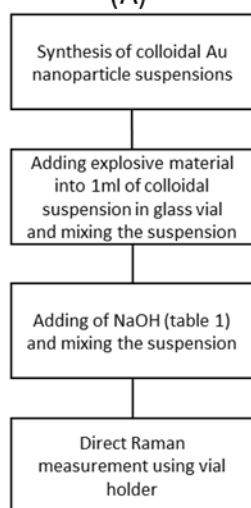


Fig. S1 Molecular structure of the explosive materials.

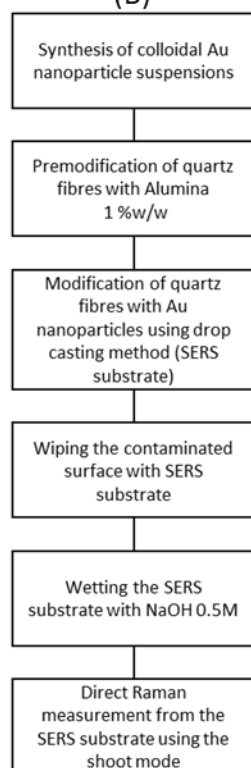
Table S1 The iterative hydroxylamine seeding method.

Colloid type	Colloidal suspension	H ₂ O	α	β	Average diameter
B	sol. A 15 ml	135 ml	1.25 ml	1.5 ml	24 nm
C	sol. B 25 ml	75 ml	0.562 ml	1.0 ml	39 nm
D	sol. C 55 ml	50 ml	0.375 ml	1.0 ml	44 nm
E	sol. A 50 ml	50 ml	0.375 ml	1.0 ml	60 nm

Analysis using nanoparticle suspension (A)

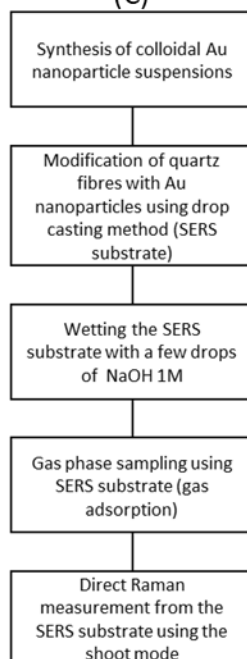


Analysis of particle samples (B)

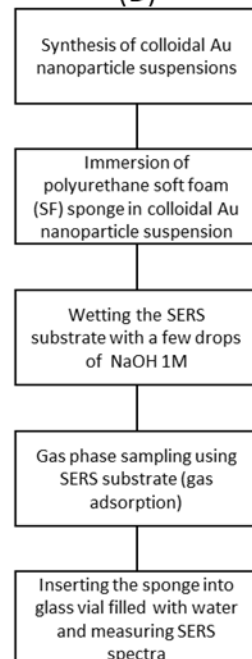


Analysis of gas phase samples

SERS measurements using Au decorated quartz fibers (C)



SERS measurements using Au decorated sponge (D)

**Fig. S2** Procedures for SERS detection of explosives in solution/gas phase/ particles on a surface.

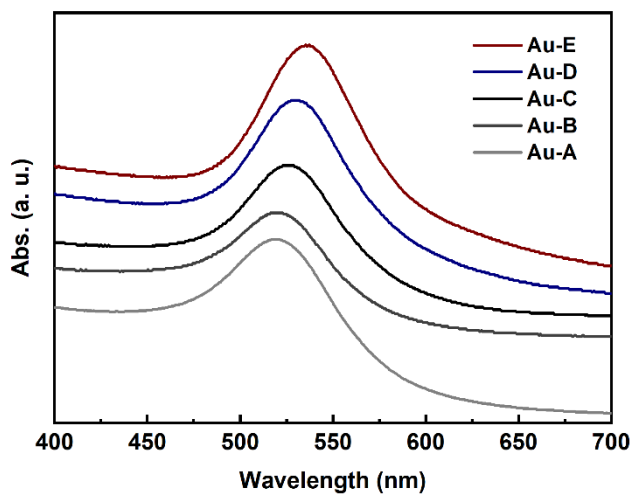


Fig. S3 UV-Vis spectra of Au colloidal suspensions Au-B to Au-E grown by iterative hydroxylamine seeding of ~12 nm diameter Au colloidal suspension (Au-A).

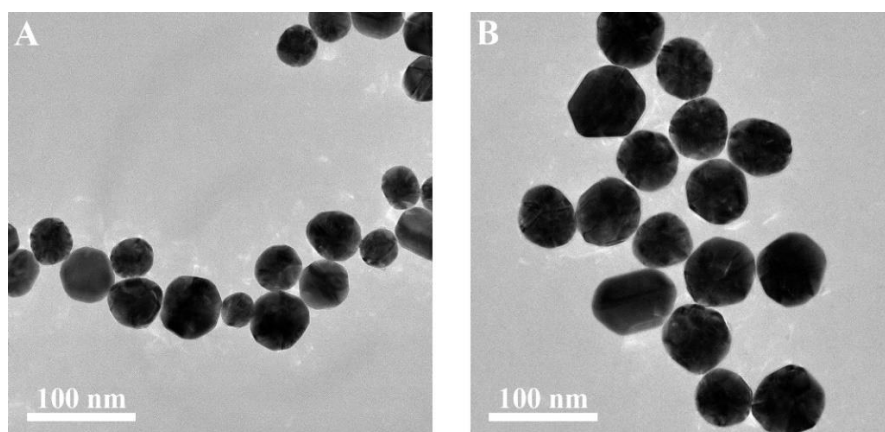


Fig. S4 Representative TEM images of the Au-D (A) and Au-E (B) nanoparticles.

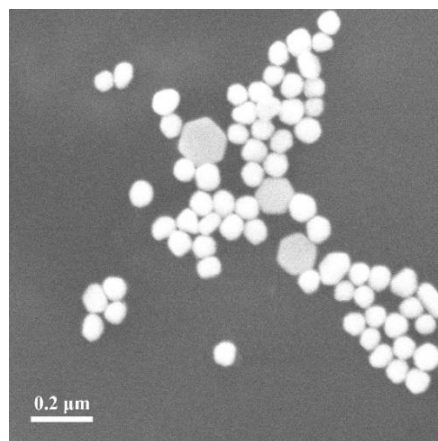


Fig. S5 Representative SEM image of the Au-Asc nanoparticles.

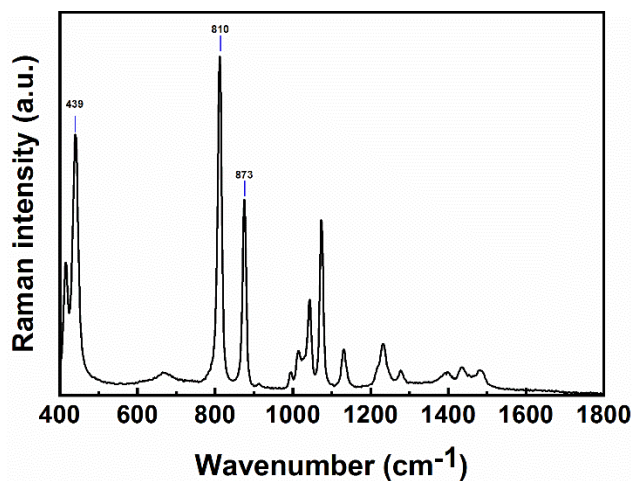


Fig. S6 Normal Raman spectrum of pentaerythritol using an accumulation time of 10 s.

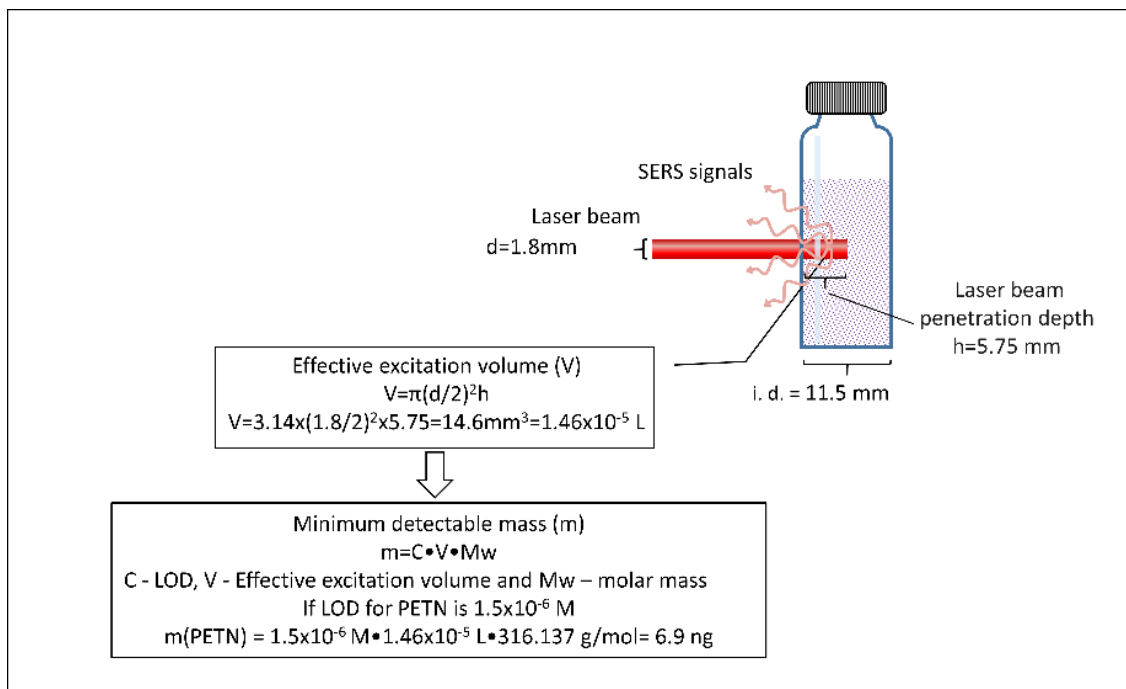


Fig. S7 Estimation of the minimum detectable mass.

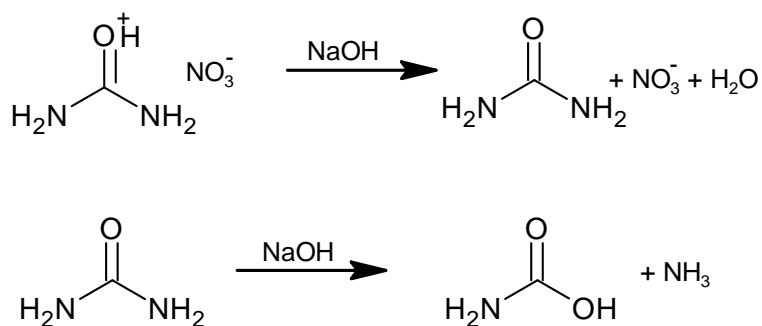


Fig. S8 Hydrolysis of UN under alkaline conditions

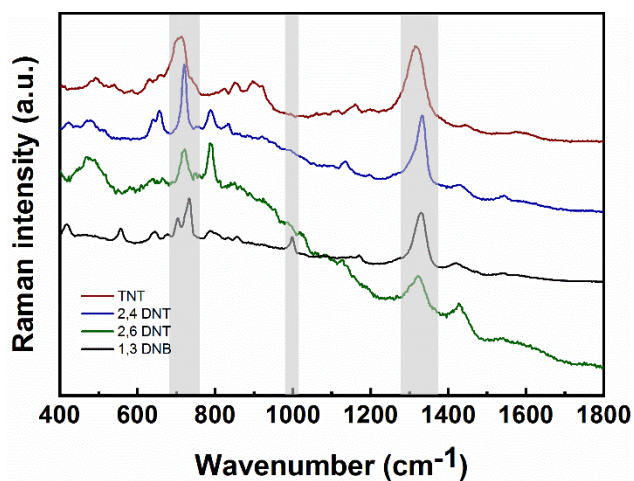


Fig. S9 Normalized SERS spectra of TNT and its impurities (2,4-DNT, 2,6-DNT, 1,2-DNB) in Au-D nanoparticle suspensions, under alkaline conditions (NaOH 36 mM).

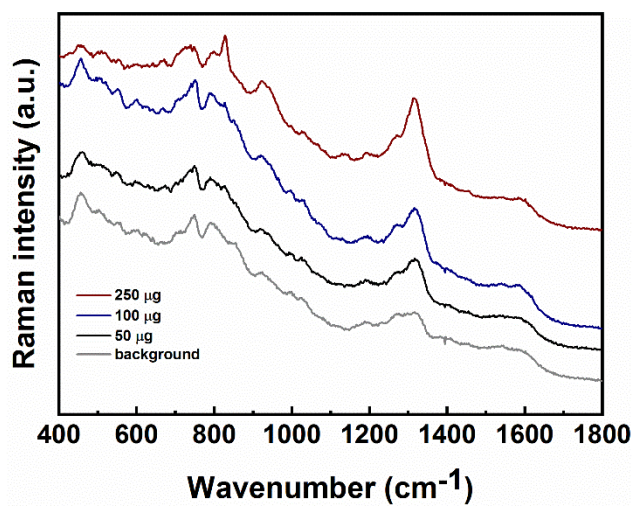


Fig. S10 Gas-phase 2,4-DNT SERS spectra obtained using sponge-based SERS substrates and an accumulation time of 5 s.

Table S2 LODs for SERS detection of explosives in solution/ gas phase/ particles on a surface.

Explosive material	Phase	LOD (experimental)	LOD (calculated)
PETN	solution	0.48 $\mu\text{g mL}^{-1}$ ($1.5 \times 10^{-6} \text{ M}$)	6.9 ng
HMX	solution	2.4 $\mu\text{g mL}^{-1}$ ($8.1 \times 10^{-6} \text{ M}$)	35 ng
UN	solution	113 $\mu\text{g mL}^{-1}$ ($9.2 \times 10^{-4} \text{ M}$)	165 ng
TNT	solution	0.024 $\mu\text{g mL}^{-1}$ ($1.1 \times 10^{-7} \text{ M}$)	0.35 ng
	particles	10 μg	0.53 $\mu\text{g cm}^{-2}$
2,4-DNT	gas phase	0.1 μg	3.6 ng
1,3-DNB	gas phase	1.5 μg	54 ng