

## Supplementary materials

### Halogen ions modified Ag NPs for ultrasensitive SERS detection of nitroaromatic explosives

Dongmei Wang<sup>a, b</sup>, Zhengjun Gong<sup>a, b\*</sup>, Mi Tang<sup>a</sup>, Wanli Fan<sup>a</sup>, Bing Huang<sup>c</sup> and Meikun Fan<sup>a, b\*</sup>

<sup>a</sup>Faculty of Geosciences and Environmental Engineering, Southwest Jiaotong University, Chengdu, China.

<sup>b</sup>State-province Joint Engineering Laboratory of Spatial Information Technology of High-Speed Rail Safety, Chengdu, 610031, China.

<sup>c</sup>Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, China.

\*Corresponding author: gongzhengjun@126.com; meikunfan@gmail.com

#### 1. Preparation of the Ag NPs

Briefly, 12 mL of 1% sodium citrate solution was quickly added to 300 mL of silver nitrate solution (1 mM), which was heated to boiling under vigorous stirring. Heating and refluxing must last for one hour to stop. After cooling to room temperature under stirring, the solution can be used as the experimental silver colloids.

#### 2. The UV-Vis absorption spectra of Ag NPs and Ag NPs modified with KI

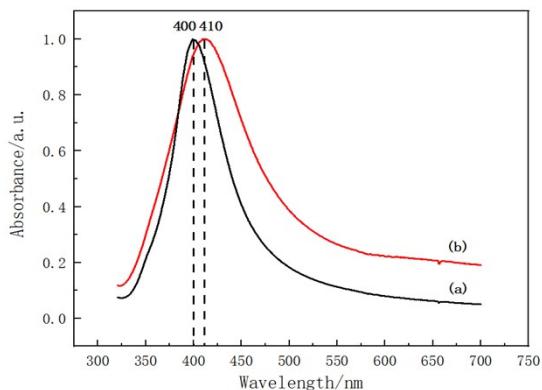


Fig. S1 The UV results of Ag NPs and Ag NPs modified with KI

### 3. DLS records of Ag NPs and Ag NPs modified with KI

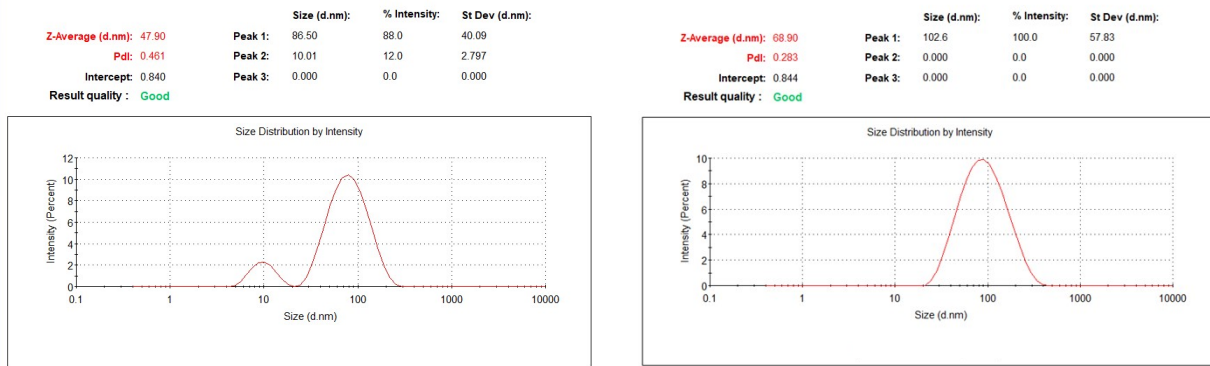


Fig S2 DLS records of Ag NPs and Ag NPs modified with KI

### 4. Table S1 SERS characteristic peak assignment of citrate

Table S1 SERS characteristic peak assignment of citrate

frequency(cm-1)		assignment
experiments	reference situation	
558	560	$\delta(\text{COO})$
597	569	$\delta(\text{COO})$
675	670	$\delta(\text{COO})$
802	800	BackBone geometry and phosphate ion interactions
920	912	$\nu(\text{C-COO})$
940	940	C-C stretch backbone
1037	1026	O-CH <sub>3</sub> stretching of methoxy groups
1287	1267	$\delta(\text{COO})$
1388	1400	$\nu(\text{C=O})\text{O}^-$ (amino acids aspartic & glutamic acid)

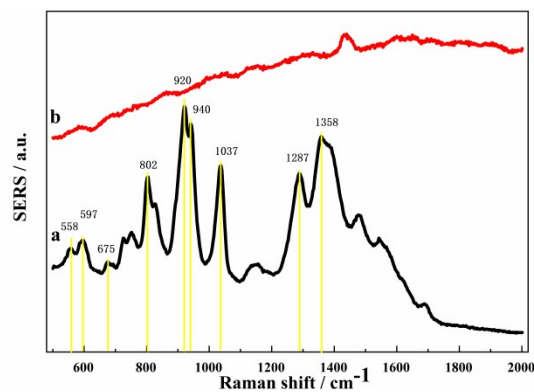
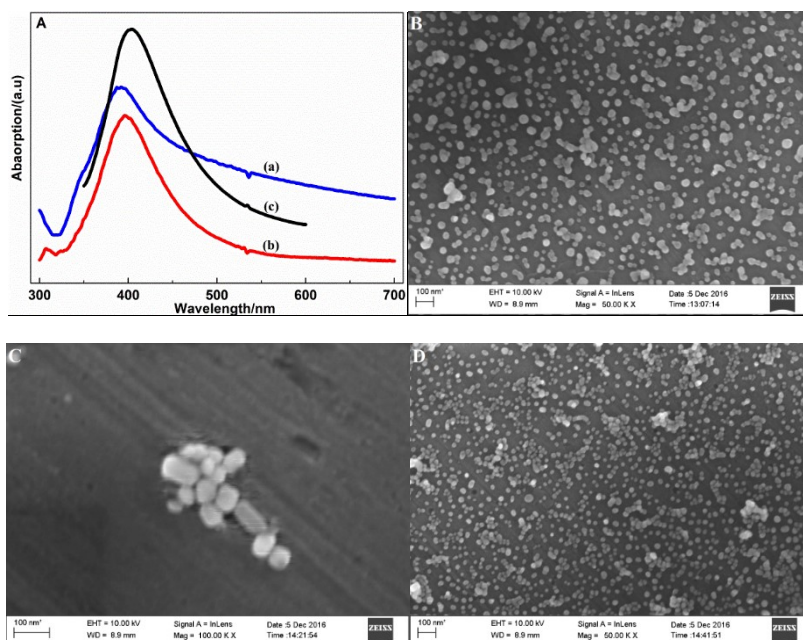


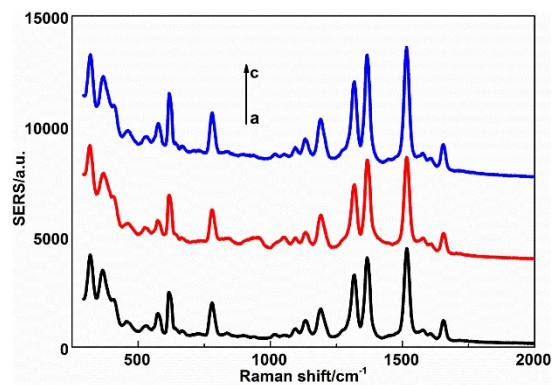
Figure S3 SERS spectra of Ag NPs

## 5. The characterization of Ag NPs



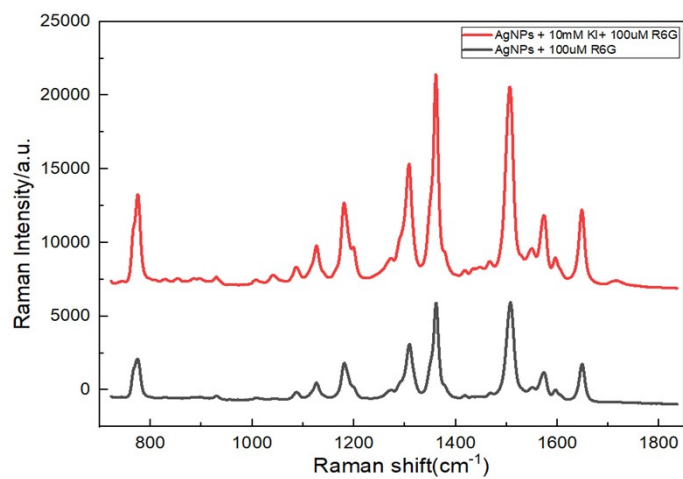
**Figure S4.** A UV spectra of Ag NPs via different reducing agent, spectra (a) to (c) were: Ag NPs (Sodium borohydride), Ag NPs (Hydroxylamine hydrochloride), Ag NPs (Sodium citrate), respectively. SEM images of: the Ag NPs prepared with (B) hydroxylamine hydrochloride, (C) sodium citrate and (D) sodium borohydride.

## 6. The SERS spectra of R6G with Ag NPs



**Figure S5.** SERS spectra of R6G obtained on Ag NPs via different reducing reagents. Spectra *a* to *c* were: Ag NPs prepared with Sodium borohydride, Sodium citrate, and Hydroxylamine hydrochloride, respectively. Sample: 5  $\mu$ L 100  $\mu$ M R6G. Integration time 5 s.

7. The comparison of the modified and unmodified nanoparticles performance towards R6G



**Figure S6.** SERS spectra of R6G obtained on Ag NPs prepared with Sodium citrate. Sample: 5  $\mu$ L 100  $\mu$ M R6G. Integration time 5 s.