Rapid detection of trace nitrobenzene in water via SERS using a portable

Raman spectrometer

Zhen-Wei Yang,*a Zhou Yu,^b Ju-Fang Zheng,*,^b Ya-Hao Wang*,^b and Xiao-Shun Zhou^b

^a Key Laboratory of Estuarine Ecological Security and Environmental Health, Tan Kah Kee College, Xiamen University, Zhangzhou 363105, China.

^b Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua 321004.

* Corresponding authors

E-mails: zwyang@xujc.com; jfzheng@zjnu.cn; yahaowang@zjnu.edu.cn

Supplementary Figures

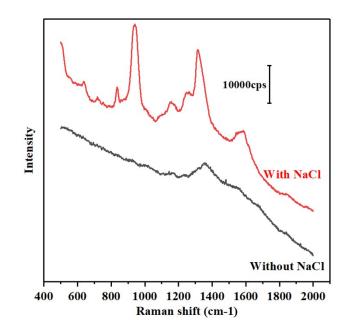


Fig. S1 SERS spectra of 0.5 mol/L TNT solution with (red line) and without (black line) NaCl solution.

We have also compared the SERS spectra with or without NaCl in Fig. S1. Obviously, in the absence of NaCl solution, the SERS spectra of TNT molecules is much weaker than that with NaCl solution. This proves that the apparent aggregation of Au nanparticle in sol induced by the NaCl to form SERS hot spots consist with many previous reports.

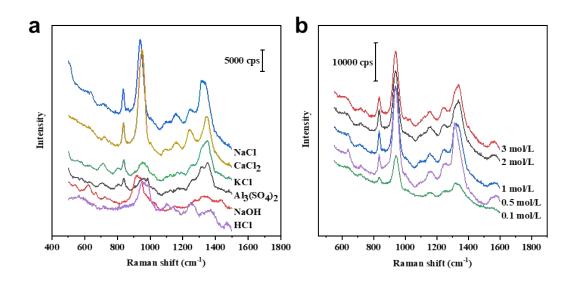


Fig. S2. SERS spectra of 0.5 mol/L TNT solution under (a) various electrolyte solutions and(b) different concentrations of NaCl solution.

In the early stages of our experiment, we have conducted screenings for different aggregating agents, including acids, bases, and salts. We tried 1 mol/L solutions of NaCl, CaCl₂, KCl, NaOH, HCl, and saturated $Al_2(SO_4)_3$ (the saturation concentration of $Al_2(SO_4)_3$ is less than 1 mol/L). It was found that the system exhibited the highest enhancement capabilities when using NaCl and CaCl₂ as aggregating agents (Fig. S2a). However, due to the tendency of Ca²⁺ to precipitate in the real water samples, we opted for NaCl solution as the aggregating agent for this detection. We further studied NaCl solutions with different concentrations, and the 1 mol/L NaCl solution produced the strongest SERS signal. (Fig. S2b). Therefore, the 1 mol/L NaCl solution was choose as the aggregating agent for this detection system.

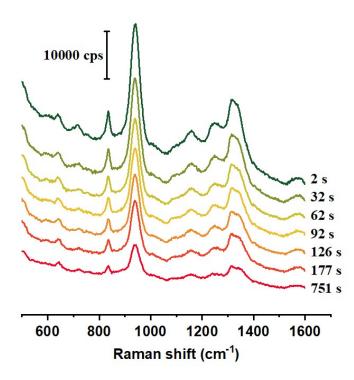


Fig S3. (a)Time-dependent SERS spectra of 0.5 mol/L TNT after the sample is added to the Au sol and shaken to mix.

Fig. S3 shows the time-dependent SERS spectra after the sample is added to the Au sol and shaken to mix. The Raman signal of TNT can be clearly distinguished even after 751 seconds, and the Raman band intensity of 834 cm⁻¹ barely changes during the first minute. Our SERS acquisition time is only 2 seconds, the extended duration of the SERS signal ensures sufficient time to detect TNT.