

Supporting Information

# A Gold Nanohole Array Based Surface-Enhanced Raman Scattering Biosensor for Detection of Silver(I) and Mercury(II) in Human Saliva

*Peng Zheng<sup>1</sup>, Ming Li<sup>1</sup>, Richard Jurevic<sup>2</sup>, Scott K. Cushing<sup>1, 3</sup>, Yuxin Liu<sup>4</sup> and Nianqiang Wu<sup>1,\*</sup>*

<sup>1</sup>Department of Mechanical and Aerospace Engineering, West Virginia University, Morgantown,  
WV 26506-6106, USA

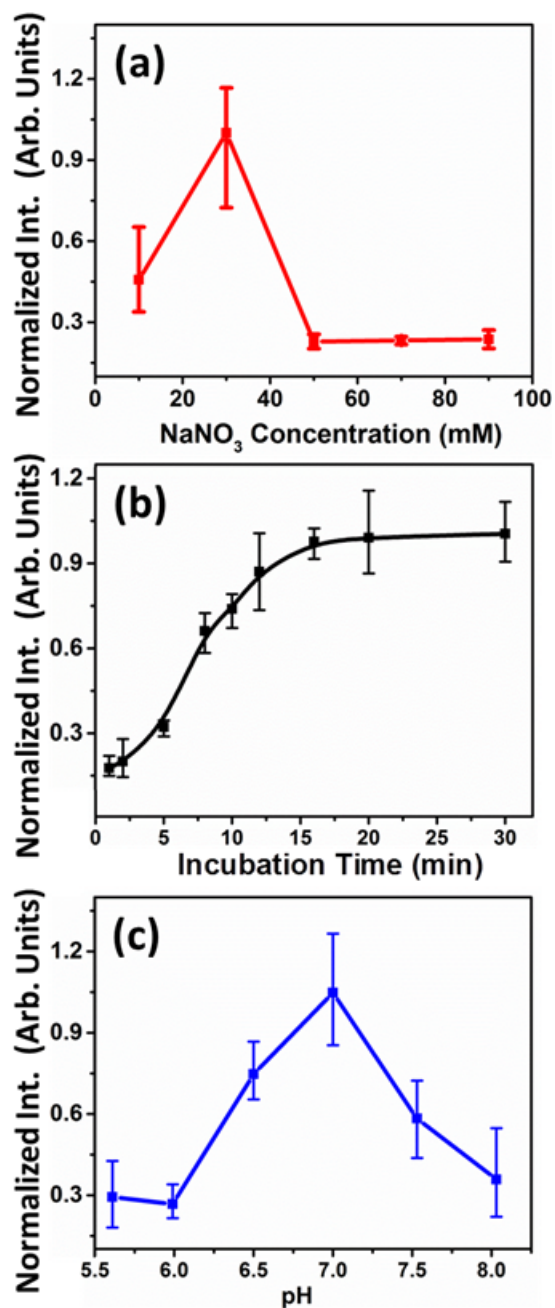
<sup>2</sup>Department of Oral Diagnostics, School of Dentistry, West Virginia University, Morgantown,  
WV 26506-9000, USA

<sup>3</sup>Department of Physics, West Virginia University, Morgantown, WV 26506-6315, USA

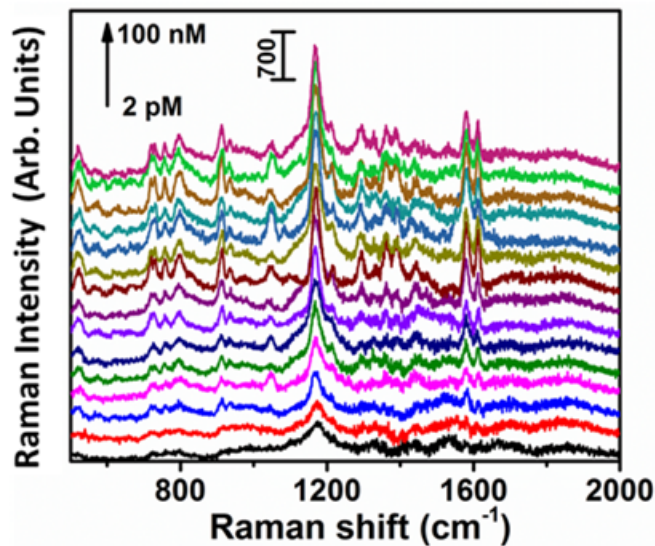
<sup>4</sup>Lane Department of Computer Science and Electrical Engineering, West Virginia University,  
Morgantown, WV 26506-6109, USA

\*To whom the correspondence should be addressed. Fax: +1-304-293-6689, E-mail:

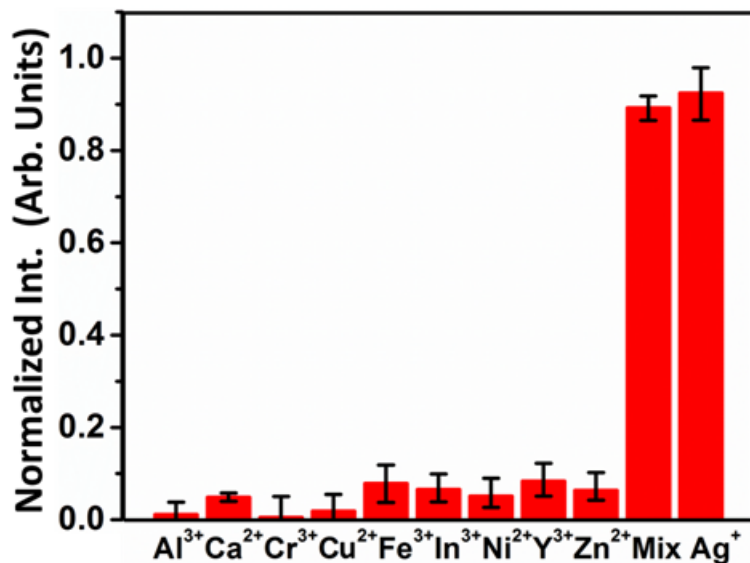
[nick.wu@mail.wvu.edu](mailto:nick.wu@mail.wvu.edu)



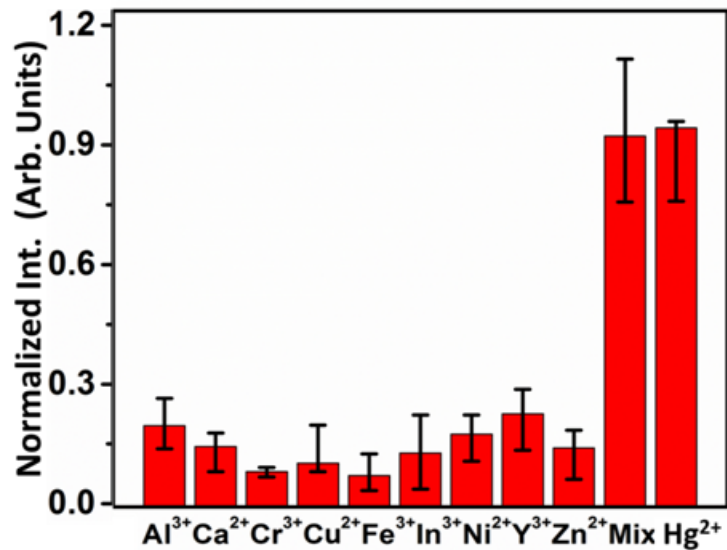
**Figure S1 Optimization of operating condition for the SERS sensor.** (a) Ionic strength optimization. The optimal ionic strength was found to be 30 mM; (b) Incubation time optimization with the optimal value of 16 min; (c) pH optimization. A neutral pH is preferred.



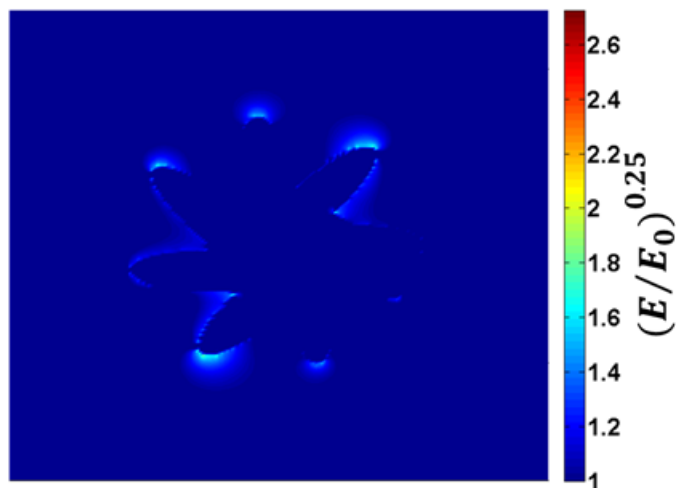
**Figure S2 SERS spectra corresponding to different levels of Ag(I) ions.** The spectra were obtained from Au nanostar@MGITC@SiO<sub>2</sub> coupled with Au film at different concentrations of Ag<sup>+</sup> ions in the MOPS buffer



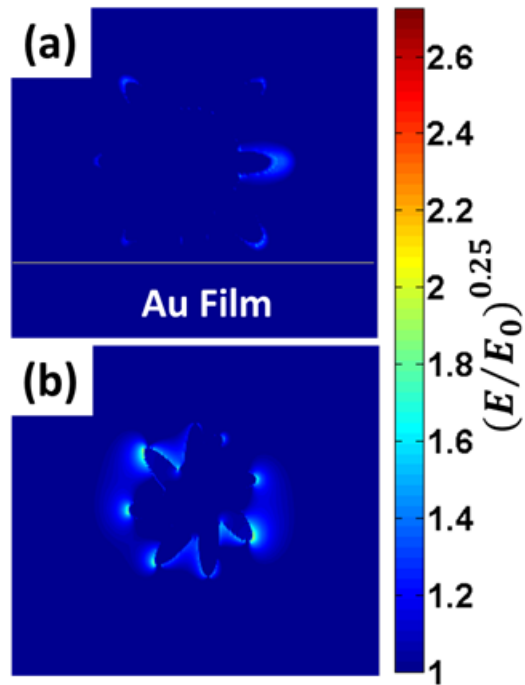
**Figure S3 Selectivity test of the Ag(I) sensor against other metal ions.** All metal ions were prepared with a concentration of 50 nM in 10 mM MOPS buffer solution containing 30 mM NaNO<sub>3</sub>. The sensor shows excellent selectivity towards silver ions in the complex mixture solution.



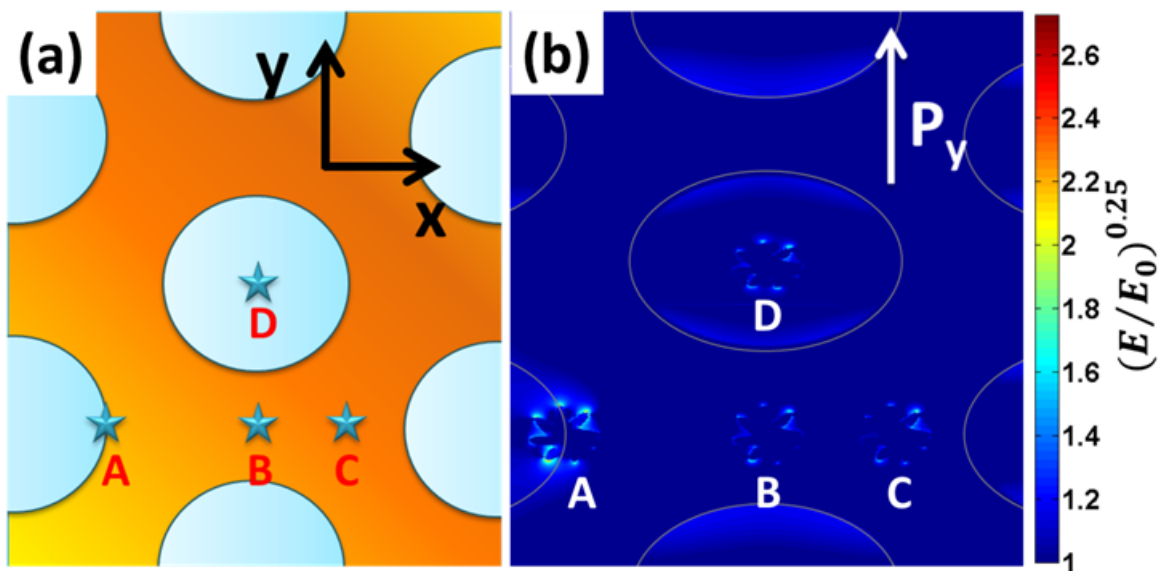
**Figure S4 Selectivity test of the Hg(II) sensor against other metal ions.** All metal ions were prepared with a concentration of 50 nM in PBS buffer. The sensor shows excellent selectivity towards mercury ions in the complex mixture solution.



**Figure S5 Simulated EM field distribution of a single Au nanostar.** The peak SERS enhancement factor  $(E/E_0)^4$  is calculated to be  $1.4 \times 10^4$ .  $(E/E_0)^{0.25}$  was used to represent the EM field enhancement for EM field enhancement for visualization purposes.

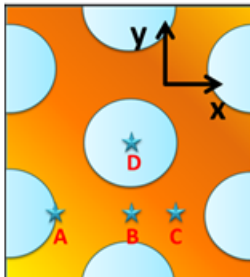


**Figure S6 Simulated EM field distributions for Au nanostar is coupled with Au film.** This geometry led to a peak SERS enhancement factor  $(E/E_0)^4$  of  $1.5 \times 10^5$ . (a) A cross-section perpendicular to Au film with the cross-section cut from the center of the Au nanostar; (b) A cross-section parallel to the Au film with the cross-section cut from the center of the Au nanostar.  $(E/E_0)^{0.25}$  was used to represent the EM field enhancement for visualization purposes.



**Figure S7 Simulated EM field distributions.** (a) FDTD simulation cell with four Au nanostars located at point A (the rim of a nanohole), point B (the gap center between two nanoholes), point C (the gap center between three nanoholes), and point D (the nanohole center); (b) simulated EM field distribution of Au nanostars on Au nanohole array at point A, B, C, and D. The simulations were conducted under y polarization with a 785 nm laser source.  $(E/E_0)^{0.25}$  was used to represent the EM field enhancement for visualization purposes.

**Table S1 SERS enhancement factors**

	Maximum SERS enhancement factors $(E/E_0)^4$ of Au nanostar at different locations on Au nanohole array			
	A	B	C	D
	$4.5 \times 10^6$	$1.0 \times 10^6$	$5 \times 10^5$	$1.1 \times 10^5$