

**Supporting Information**

**Mercury Species Induced Frequency-Shift of Molecular Orientational  
Transformation Based on SERS**

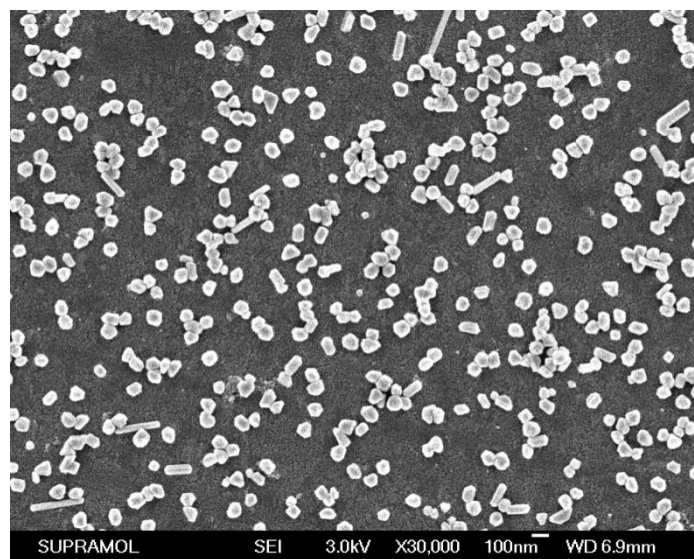
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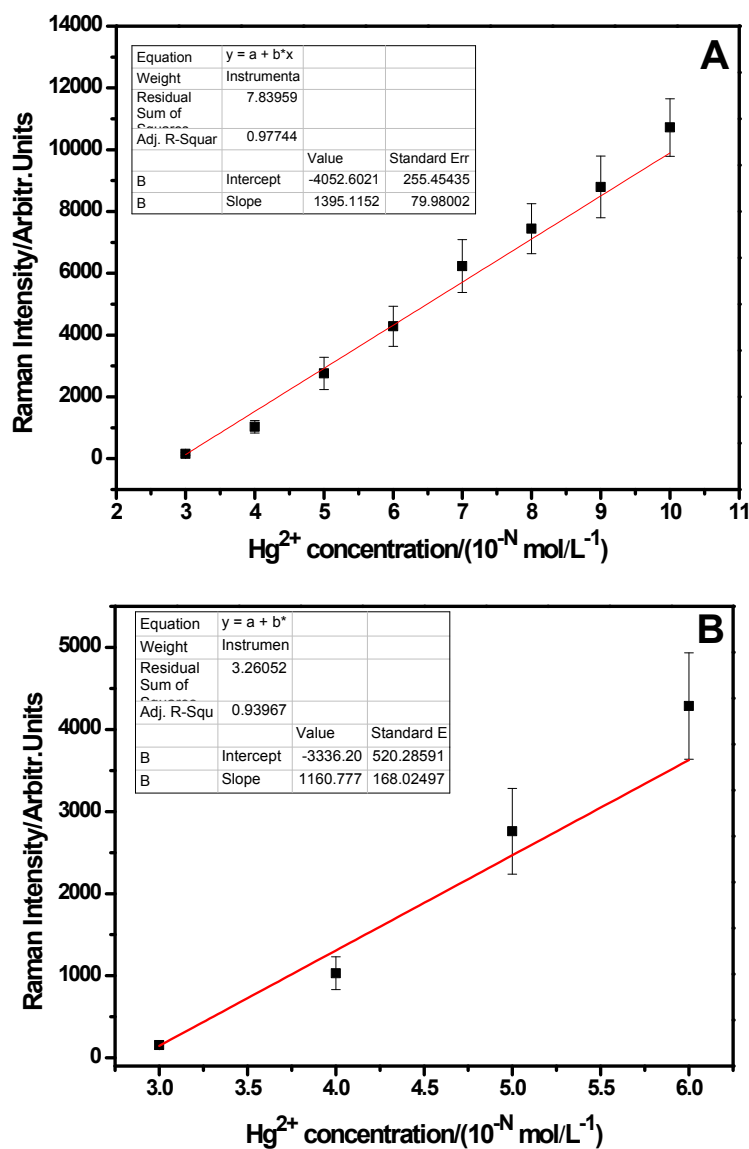
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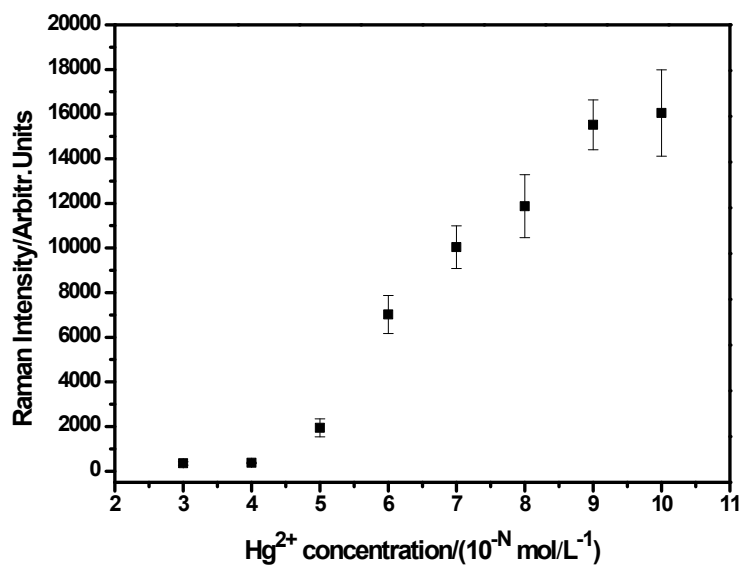
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[hanxiaoxia@jlu.edu.cn](mailto:hanxiaoxia@jlu.edu.cn).



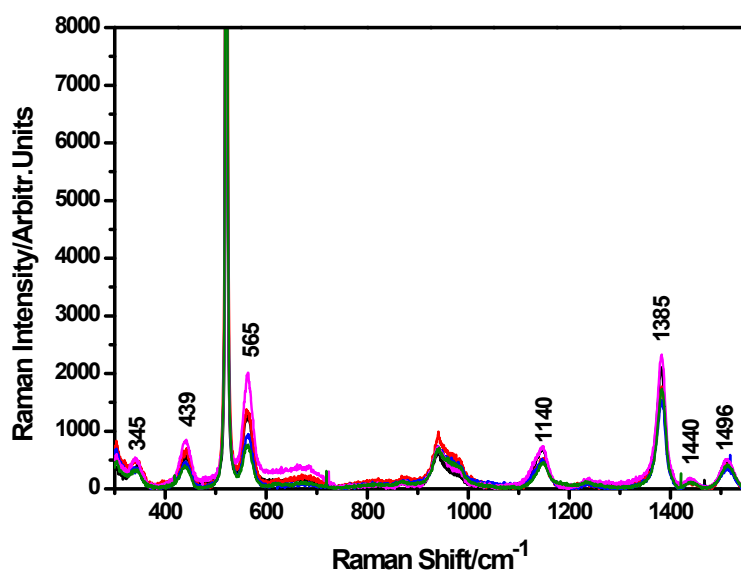
**SI\_Figure 1.** SEM image of self-assemble silver colloid film.



**SI\_Figure 2.** (A) Concentration-dependent SERS spectra of DASS with  $\text{Hg}^{2+}$  concentration range from  $10^{-3}$  to  $10^{-10}$  mol/L. The standard curve of the standard solution ( $\text{Hg}^{2+}$ ) obeys the equation  $Y = 1395.12X - 4052.60$ ,  $R^2 = 0.9774$ , where  $Y$  represents the SERS intensities of the band at  $1375 \sim 1389 \text{ cm}^{-1}$  of DASS, and  $X$  is the concentration of  $\text{Hg}^{2+}$ . (B) Concentration-dependent SERS spectra of DASS with  $\text{Hg}^{2+}$  concentration range from  $10^{-3}$  to  $10^{-6}$  mol/L. The standard curve of the standard solution ( $\text{Hg}^{2+}$ ) obeys the equation  $Y = 1160.78X - 3336.20$ ,  $R^2 = 0.9397$ , where  $Y$  represents the SERS intensities of the band at  $1378 \sim 1389 \text{ cm}^{-1}$  of DASS, and  $X$  is the concentration of  $\text{Hg}^{2+}$ .



SI\_Figure 3. (A) Concentration-dependent SERS spectra of DASS (band at 565 cm<sup>-1</sup>) with Hg<sup>2+</sup> concentration range from 10<sup>-3</sup> to 10<sup>-10</sup> mol/L.

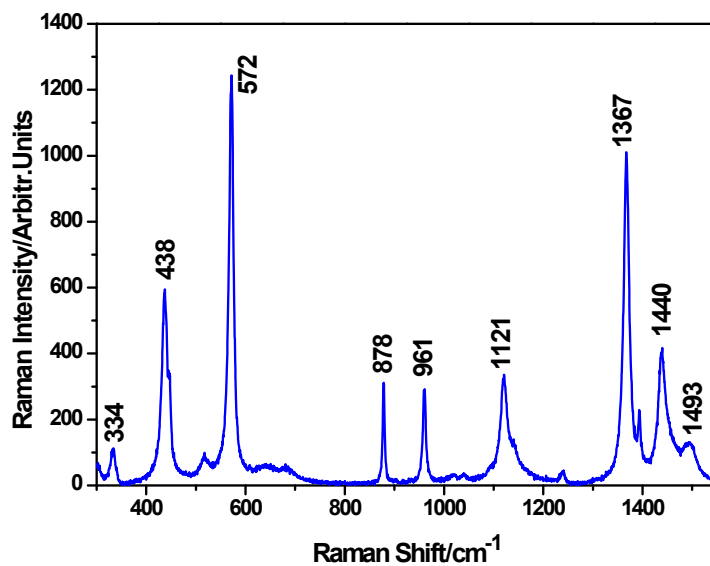


SI\_Figure 4. SERS spectra of DASS in the presence of the mercury ions at a concentration of 10<sup>-4</sup> mol/L on five different chips. The DASS-modified silver nanoparticles used as a sensor chip indeed provided rather irreproducible SERS intensity due to irreproducible distribution of hot spot and possible aggregation of nanoparticles.

**SI\_Table 1.** Mean wavenumbers ( $\text{cm}^{-1}$ ) of the Raman and SERS spectra of DASS.

Raman ( $\text{cm}^{-1}$ )	SERS( $\text{cm}^{-1}$ )	Assignment
334	345	$\delta(\text{S}=\text{CS})$
438	439	$\delta(\text{CH}_3\text{NC}), \nu(\text{C}=\text{S})$
572	565	$\nu(\text{CSS})$
878	876	$\nu(\text{CH}_3\text{N})$
961	947	$\nu(\text{CH}_3\text{N}), \nu(\text{C}=\text{S})$
1121	1140	$\rho(\text{CH}_3), \nu(\text{CN})$
1367	1374~1389	$\delta_s(\text{CH}_3), \nu(\text{CN})$
1440	1440	$\delta_{\text{as}}(\text{CH}_3), \nu(\text{CN})$
1493	1496	$\nu(\text{CN}), \delta(\text{CH}_3),$ $\rho(\text{CH}_3)$

$\nu$ =stretching,  $\delta$ = deformation,  $\rho$ = rocking



**SI\_Figure 5.** Raman spectrum of DASS powder.