

Figure S1. TEM images of (A) AuNS and (B) AuNS@Ag. (C) EDS spectra of AuNS@Ag and AuNS. (D) XRD patterns of AuNS@Ag and AuNS.

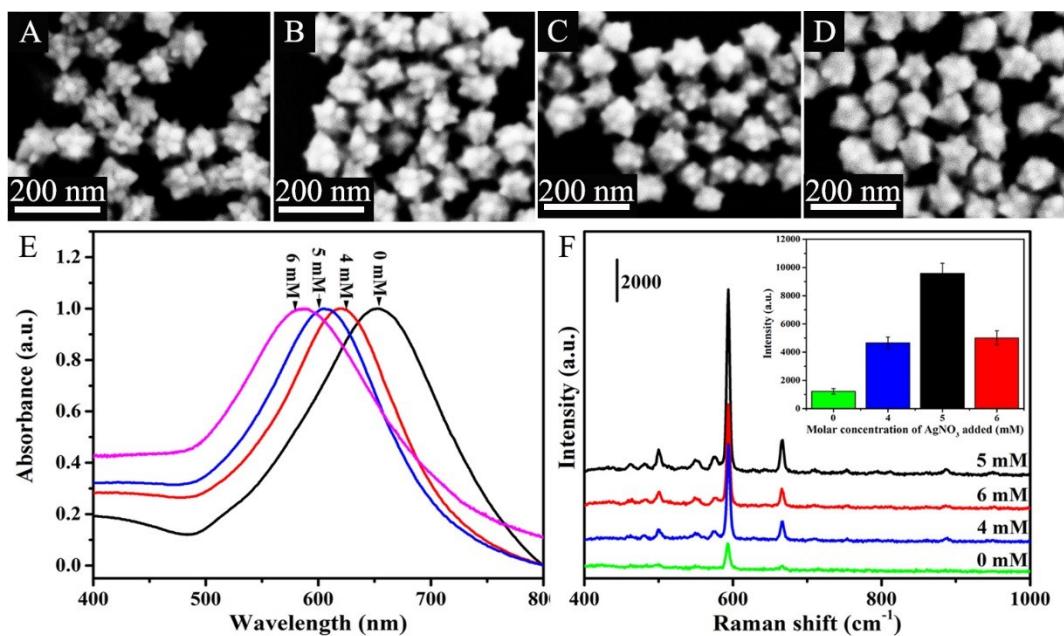


Figure S2. SEM images of the obtained AuNS@Ag under various amounts of AgNO₃: (A) 0 mM, (B) 4 mM, (C) 5 mM, and (D) 6 mM. (E) UV-vis spectra of AuNS@Ag suspension. (F) The comparision of SERS intensity using four AuNS@Ag solutions (NBA with concentration at 10⁻⁶ M). The inset depicts the dependence of SERS intensity on concentration of AgNO₃ added, error bars indicate the standard deviation from 5 spectra.

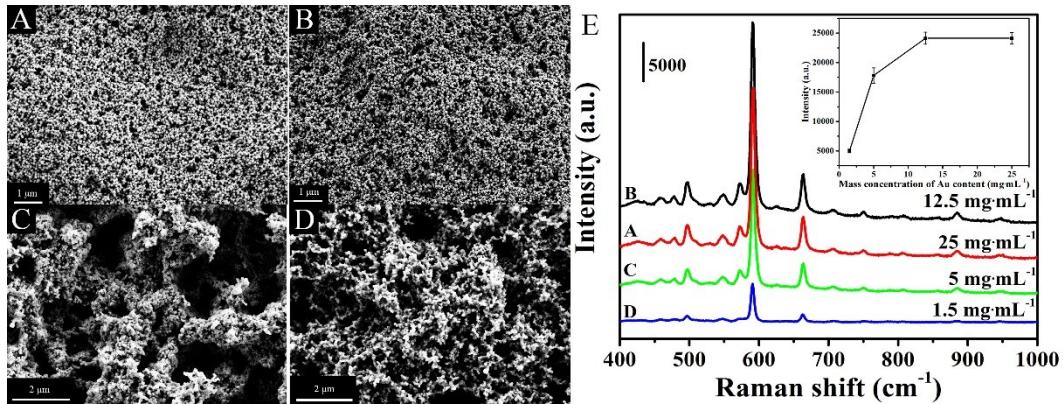


Figure S3. SEM images of AuNS@Ag/SMCSL substrate fabricated by evaporating 10 μL of AuNS@Ag with different mass concentration of Au content: (A) 25 $\text{mg}\cdot\text{mL}^{-1}$; (B) 12.5 $\text{mg}\cdot\text{mL}^{-1}$; (C) 5 $\text{mg}\cdot\text{mL}^{-1}$; (D) 1.5 $\text{mg}\cdot\text{mL}^{-1}$. (E) SERS spectra of NBA absorbed on aforementioned substrates. The inset shows the dependence of signal intensity (592 cm^{-1}) on mass concentration of Au content, error bars indicate the standard deviation from 5 spectra.

Table S1. Main SERS Band Assignments of OPD¹.

SERS/cm ⁻¹	Assignment
1157	C-H in-plane bend
1270	C-H stretching in the benzenoid
1333	C-H in-plane bend
1422	Ring deformation, C-H in-plane bend
1502	Ring deformation, C-H in-plane bend
1602	NH ₂ scissor

Table S2. Main SERS Band Assignments of 6-TG².

SERS/cm ⁻¹	Assignment
821	$\delta^{5,6}_{\text{ring}}(20) + \delta^{\text{out}}_{\text{N9C1'}}(18) + \delta^{\text{out}}_{\text{ribose}}(10) + \delta^{\text{out}}_{\text{C2'}-O2'}(9)$ + vN9-C1'(6) + vC8-N9(6)
900	$\delta^{5,6}_{\text{ring}}(45) + vC5-N7(9) + vN3-C4(8) + vC6=S(6)$
928	$\delta^{\text{out}}_{\text{C8H8}}(88)$
1016	vC1'-C2'(20) + $\delta^5_{\text{ring}}(11) + \delta^{\text{rock}}_{\text{C5'H}_2}(9) + \delta_{\text{C2'H}}(45)$
1265	$\delta_{\text{C8H8}}(40) + \delta^{5,6}_{\text{ring}}(16) + vN9-C1'(7) + vN7-C8(5)$ vC8-N9(19) + $\delta_{\text{C1'H}}(16)$ + vN9-C1'(11) + vC5-N7(6) + vN1-C2(5)
1297	$\delta_{\text{C2H2}}(28) + vC5-N7(25) + \delta^6_{\text{ring}}(10) + vN7-C8(8) + vC2-$ N3(8) + vC4-C5(7)
1387	$\delta^{\text{sciss}}_{\text{C5'H}_2}(98)$
1495	vN3-C4(38) + vC4-C5(14) + vC4-N9(12) + vN7-C8(9) + $\delta^6_{\text{ring}}(9)$ + vC2-N3(7) + $\delta_{\text{N1H1}}(6)$
1589	

Table S3. Main SERS Band Assignments of HGB³.

SERS/cm ⁻¹	Assignment
910	$\gamma (=C_bH_2)_s$
1121	$N5(C_\beta\text{-methyl stretch})$
1209	ν_{13}
1316	$\delta(C_aH=)_4$
1341	ν_{41}
1443	$\delta (=C_bH_2)_s$
1580	ν_{37}
1621	$\nu(C_a=C_b)$

Reference

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- 3 G. Smulevich and T. G. Spiro, *J. Phys. Chem.*, 1985, **89**, 5168-5173.