

Supporting information

for

Regulated Synthesis of Au NB-DT@Ag Bimetallic Core-Molecule-Shell Nanostructure for Reliable SERS Detection.

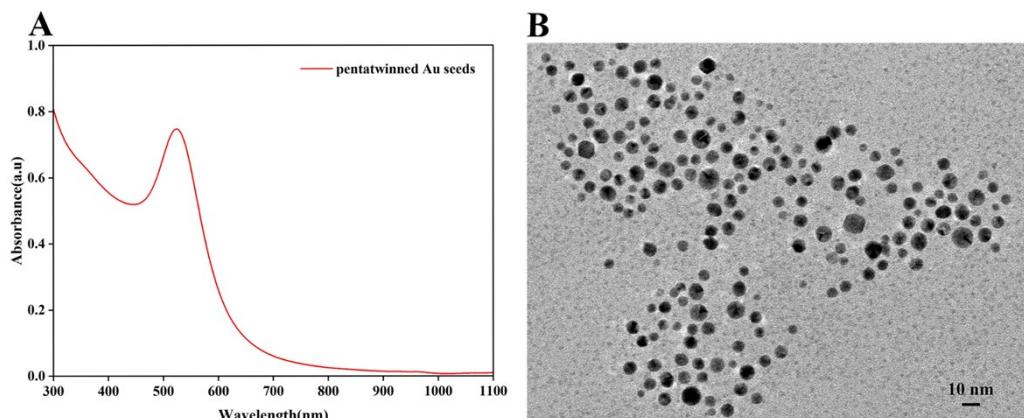


Figure S1. (A) UV-vis spectrum of Au seeds and (B) TEM image of Au seeds.

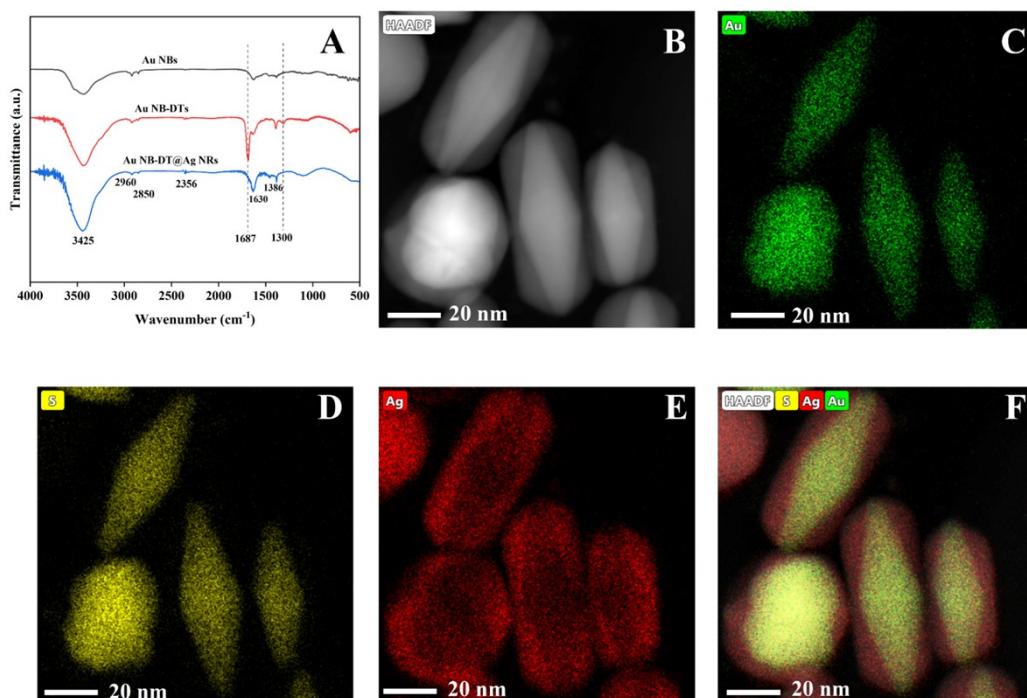


Figure S2. (A) FTIR spectra of Au NBs, Au NB-DTs and Au NB-DT@Ag NRs; (B-F) TEM images and elements mapping of Au NB-DT@Ag NRs;

Table S1: Comparison of enhancement factors of Au@Ag core-shell SERS base materials in recent years

Substrate	Analyte	AEF	Ref
Au @Fe ₃ O ₄ NPs	MG	1.10×10 ⁵	1
Ag/PDMS	MG	2.06×10 ⁵	2
Au NP@GQDs	MG	1.70×10 ³	3
ZnO NR@Au	MG	5.30×10 ⁵	4
Fe ₃ O ₄ @Ag	MG	1.00×10 ⁵	5
Au NB-DT@Ag NRs	MG	3.73×10 ⁵	This work

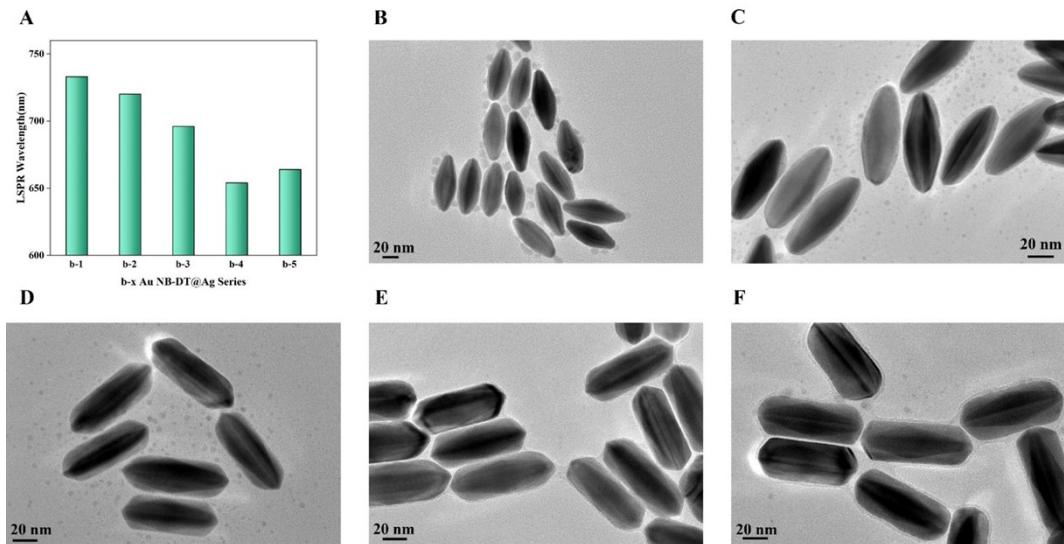


Figure S3: UV-vis spectra and TEM images of Au NB-DT@Ag NRs with controlled Ag shell thickness; (A) UV-vis spectra of b-1~b-5 Au NB-DT@Ag NRs; (B~F) TEM images of Au NB-DT@Ag NRs (B) b-1; (C) b-2 ; (D) b-3 ; (E) b-4 ; (F) b-5 ;

Table S2: Comparison of the Au NB-DT@Ag with recent reported SERS substrates used for the analysis of MG

SERS Substrate	Analyte	LOD (mol/L)	AEF	Ref
Ag-coated PDMS	MG	1.0×10^{-7}	2.06×10^5	2
Au@Ag NCs	MG	5.0×10^{-9}	-	6
Au NP/HMM	MG	1.0×10^{-8}	1.56×10^5	7
Au Nanowires	MG	1.0×10^{-6}	-	8
Au NPs/GDY/CC	MG	1.0×10^{-9}	5.4×10^5	9
Au-coated ZnO NRs	MG	5.0×10^{-9}	5.3×10^5	10
Fe ₃ O ₄ @Au MCS	MG	1.0×10^{-7}	1.10×10^5	11
Au NB-DT@Ag NRs	MG	5.0×10^{-9}	3.73×10^5	This work

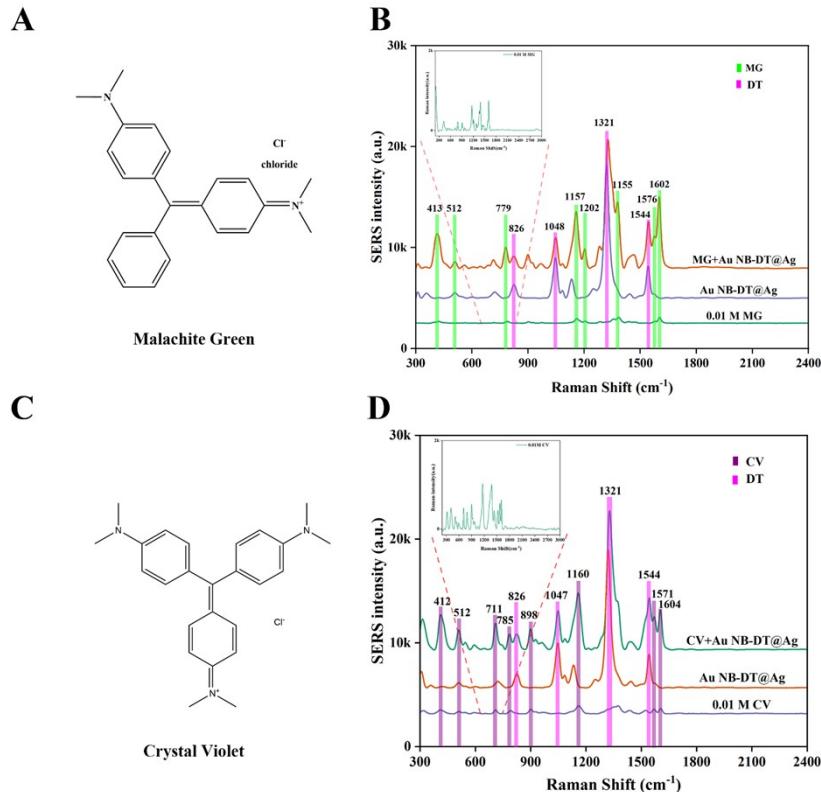


Figure S4. (A) Molecule structures of MG; (B) Raman spectra of Au NB-DT@Ag NRs and Au NB-DT@Ag NRs+MG and 0.01M MG solution, insected the Raman spectrum of MG (C) Molecule structures of CV; (D) Raman spectra of Au NB-DT@Ag NRs and Au NB-DT@Ag NRs+CV and 0.01M CV solution, insected the Raman spectrum of CV.

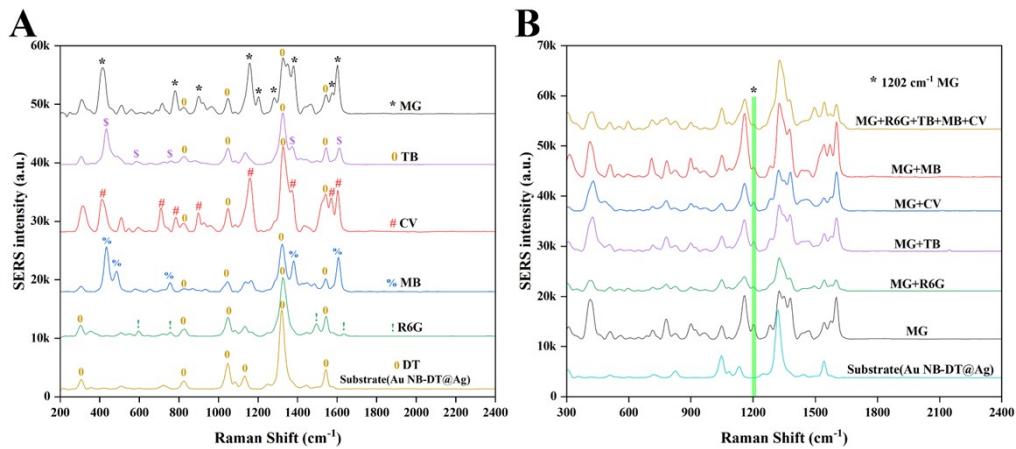


Figure S5. (A) SERS spectra of MG, TB, CV, MB and R6G with the substrate (Au NB-DT@Ag). (B) SERS spectra of MG+MB, MG+CV, MG+TB, MG+R6G mixtures, MG with the substrate and the blank substrate.

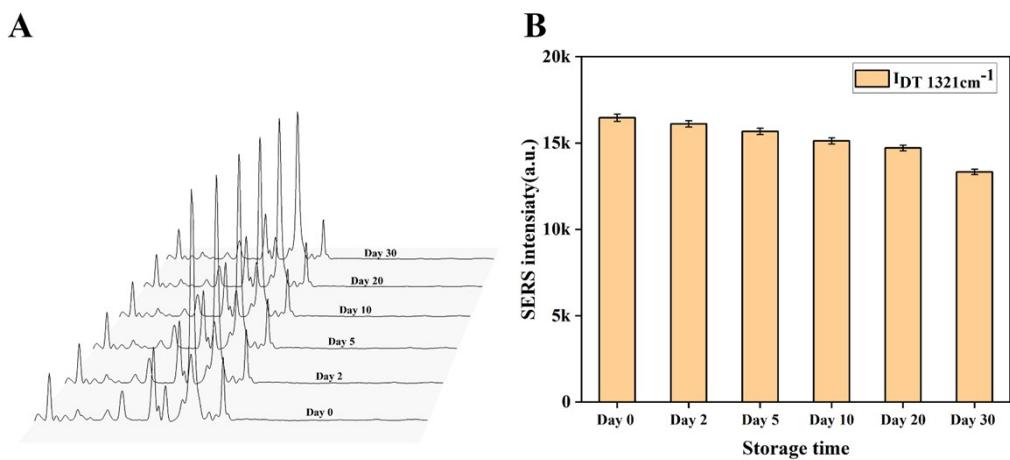


Figure S6: (A) SERS intensity of DT at 1321 cm⁻¹ under different storage time; (B) Histogram of SERS intensity of 1321 cm⁻¹ of different storage time.

Table S3 Assignments of Raman and SERS peaks of DT, MG and CV on the substrate

Molecule	Raman peak position(cm ⁻¹)	SERS peak position(cm ⁻¹)	Assignment	
DT	1062	1047	CH ₃ rocking	¹²
	1150	1131	C-N stretching; C-N bending	
	1333	1326	Symmetric NO ₂ stretching	
	1556	1544	Aromatic ring stretching	
MG	424	413	C-phenyl out-of-plane bending	^{2, 3}
	518	512		
	780	779	C-H out-of-plane bending	
	903	898	C-H out-of-plane bending	
	1160	1157	C-H in-plane bending in ring	
	1206	1202	C-H in-plane bending in ring	
	1579	1576	N-phenyl stretching bending	
	1602	1602	Ring C-C stretching vibration	
CV	412	412	C-N-C bending	¹³
	517	512	C-N-C bending	
	711	711	C-N-C symmetric stretching	
	790	785	Ring C-H bending	
	903	898	Phenyl ring breathing mode	
	1160	1160	C-phenyl C-H in-plane stretching	
	1575	1572	Ring C-C stretching	
	1606	1604	Ring C-C stretching	

Reference

1. Z. H. Li, J. H. Bai, X. Zhang, J. M. Lv, C. S. Fan, Y. M. Zhao, Z. L. Wu and H. J. Xu, *Spectrochim Acta A Mol Biomol Spectrosc*, 2020, **241**, 118532-118539.
2. P. Kumar, R. Khosla, M. Soni, D. Deva and S. K. Sharma, *Sensors and Actuators B: Chemical*, 2017, **246**, 477-486.
3. X. Fei, Z. Liu, Y. Li, G. Yang, C. Su, H. Zhong, Z. Zhuang and Z. Guo, *Journal of Alloys and Compounds*, 2017, **725**, 1084-1090.
4. B. Li, Y. E. Shi, J. Cui, Z. Liu, X. Zhang and J. Zhan, *Analytica Chimica Acta*, 2016, **923**, 66-73.
5. X.-Y. Zhao, G. Wang and M. Hong, *Materials Chemistry and Physics*, 2018, **214**, 377-382.
6. J. Li, Q. Wang, J. Wang, M. Li, X. Zhang, L. Luan, P. Li and W. Xu, *Analytical and Bioanalytical Chemistry*, 2021, **413**, 4207-4215.
7. Z. Wang, Y. Huo, T. Ning, R. Liu, Z. Zha, M. Shafi, C. Li, S. Li, K. Xing, R. Zhang, S. Xu, Z. Li and S. Jiang, *Journal*, 2021, **11**.
8. A. La Porta, M. Grzelczak and L. M. Liz-Marzán, *ChemistryOpen*, 2014, **3**, 146-151.
9. S. Yao, Y. Lv, Q. Wang, J. Yang, H. Li, N. Gao, F. Zhong, J. Fu, J. Tang, T. Wang and D. Jia, *Applied Surface Science*, 2023, **609**, 155098.
10. B. Li, Y.-e. Shi, J. Cui, Z. Liu, X. Zhang and J. Zhan, *Analytica Chimica Acta*, 2016, **923**, 66-73.
11. Z. H. Li, J. H. Bai, X. Zhang, J. M. Lv, C. S. Fan, Y. M. Zhao, Z. L. Wu and H. J. Xu, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2020, **241**, 118532.
12. Y. Li, L. Jiang, Y. Zou, Z. Song and S. Jin, *Applied Surface Science*, 2021, **540**, 148381-148389.
13. G. Shi, M. Wang, Y. Zhu, Y. Wang and H. Xu, *Applied Surface Science*, 2018, **459**, 802-811.