

Supporting information

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2 **Highly Porous Gold Supraparticles as Surface-enhanced Raman** 3 **Spectroscopy (SERS) Substrates for Sensitive Detection of** 4 **Environmental Contaminants**

5 Seju Kang^{a,b*}, Wei Wang^{a,b}, Asifur Rahman^{a,b}, Wonil Nam^c, Wei Zhou^c, Peter J. Vikesland^{a,b*}

6 ^aDepartment of Civil and Environmental Engineering, Virginia Tech, Blacksburg, Virginia;

7 ^bVirginia Tech Institute of Critical Technology and Applied Science (ICTAS) Sustainable
8 Nanotechnology Center (VTSuN), Blacksburg, Virginia;

9 ^cDepartment of Electrical and Computer Engineering, Virginia Tech, Blacksburg, Virginia;

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11 * Corresponding authors: seju@vt.edu, pvikes@vt.edu

12 Postal address: 415 Durham, Virginia Tech, Blacksburg 24061, VA, USA

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19 **Total Pages: 5**

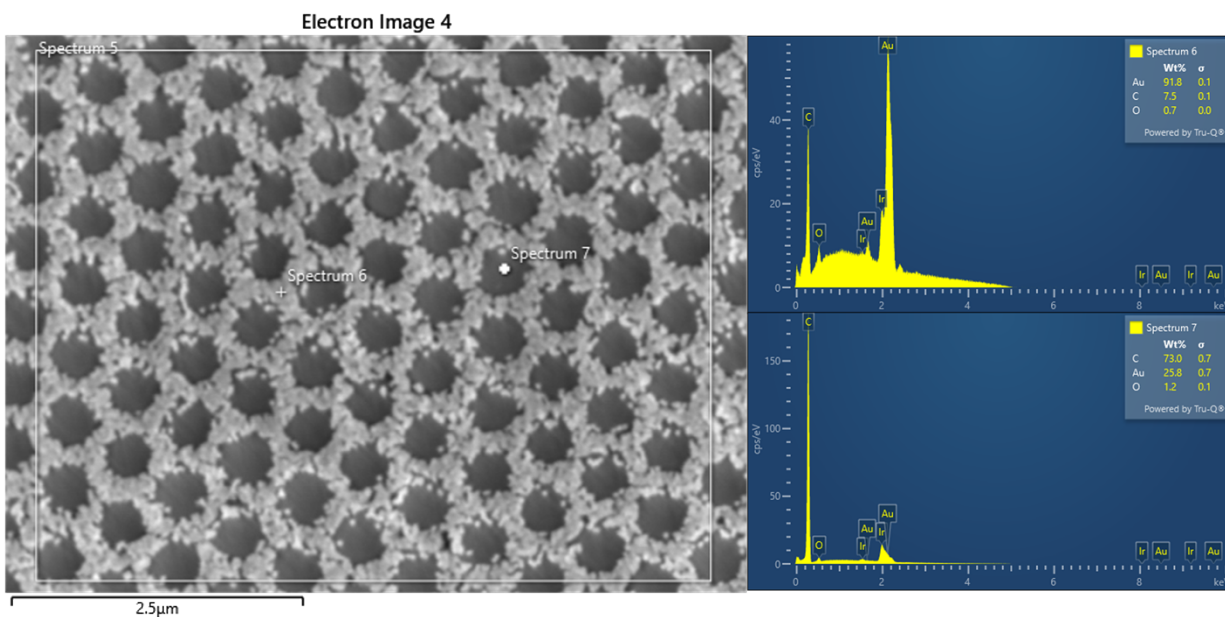
20 **Figures S3 Pages S2**

21 **Tables S1-S3 Pages S3-S4**

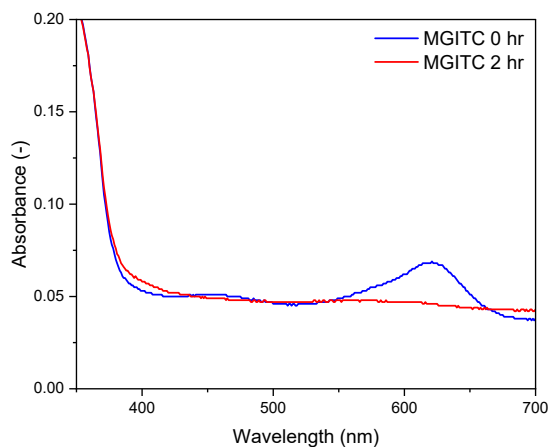
22 **SI References Page S5**

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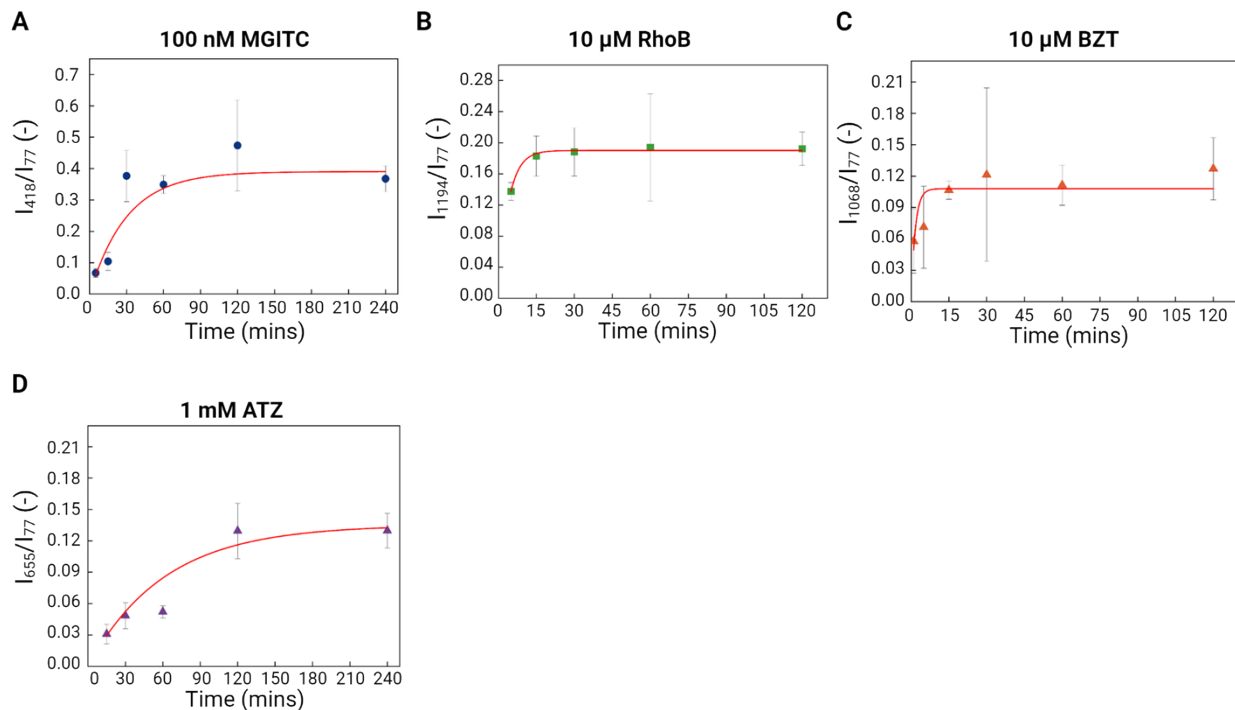
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 26 **Figure S1.** Energy dispersive spectroscopy (EDS) spectra of the Au/PS supraparticle from two
 27 different positions; a polystyrene (PS) nanoparticle and Au nanoparticle aggregates. The mass
 28 percent of Au and C, a representative of PS from EDS spectra.
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 31 **Figure S2.** Absorbance spectra of MGITC solution before and after 2 hrs of contact with the
 32 porous Au supraparticle.
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36 **Figure S3.** (A)-(D) Sorption kinetics of environmental contaminants (100 nM MGITC, 10 μ M
 37 RhoB, 10 μ M BZT, 1 mM ATZ) based on the Raman intensity increases of their characteristic
 38 peaks with time. The symbols and error bars indicate the means and standard deviation of the
 39 normalized Raman signals from the 400 SERS spectra.

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62 **Table S1.** Gene sequences for *intI1*

5'- sequences -3'	
<i>intI1</i>	GTGCACGGGCATGGTGGCTGAAGGACCAGGCCGAGGGCCGCA CGGCGTTGCGCTTCCCGACGCCCTTGAGCGGAAGTATCCGCGC

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66 **Table S2.** SERS peaks and corresponding assignments

Wavenumber (cm ⁻¹)	Assignments	ref
MGITC		
418	Out-of-plane benzene ring deformation	1
1171	In-plane benzene ν_9 mode	2
1364	The aromatic ring stretching mode	2
1388	In-plane C-C/C-H stretch	3
RhoB		
1194	C-C bridge band stretching	4
1279	Aromatic C-H bending aromatic	4
1506	Aromatic C-C bending	5
BZT		
419	C-S stretching, C-C-C ring bending (ring breathing)	6
994	C-H ring bending	6
1021	C-C-C bending and C-S stretching	6
1068	C-C-C bending and C-S stretching	6
ATZ		
655	Asymmetric deformation N-C-N/C-N-C and ring breathing	7
961	Asymmetric deformation N-C-N/C-N-C and ring breathing	7
Gene segment		
730	Adenine	8
959	Deoxyribose	9
1315	Guanine	10
1335	Adenine	8
1458	Deoxyribose	10

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72 **Table S3.** The composition of wastewater influent

pH	Na ⁺	Mg ²⁺	Si ⁴⁺	P ⁺	K ⁺	Ca ⁺
6.51	158.27 ± 5.01	6.58 ± 0.37	8.06 ± 0.70	6.10 ± 0.30	16.67 ± 0.27	12.38 ± 0.41
Specific Conductivity (μS/cm)	F ⁻	Cl ⁻	NO ²⁻	PO ₄ ³⁻	SO ₄ ²⁻	Br ⁻
1172.0	0.10 ± 0.01	135.39 ± 0.02	0.35 ± 0.02	5.74 ± 0.08	21.76 ± 0.28	0.12 ± 0.00
Total organic carbon (TOC, mg/L)						
5.38						

73 The cation and anion compositions were analyzed by using inductively-coupled plasma-mass
 74 spectrometer (ICP-MS) and ion chromatography (IC). The sample was filtered through 0.45 μm
 75 polytetrafluoroethylene (PTFE) filter.

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93 References

- 94 1 A. Kamińska, I. Dziecieliwski, J. L. Weyher, J. Waluk, S. Gawinkowski, V. Sashuk, M.
95 Fiałkowski, M. Sawicka, T. Suski, S. Porowski and R. Hołyst, *J. Mater. Chem.*, 2011, **21**,
96 8662.
- 97 2 M. Li, J. Zhang, S. Suri, L. J. Sooter, D. Ma and N. Wu, *Anal. Chem.*, 2012, **84**, 2837–
98 2842.
- 99 3 W. Leng and P. J. Vikesland, *Langmuir*, 2014, **30**, 8342–8349.
- 100 4 S. Aghajani, A. Accardo and M. Tichem, *ACS Appl. Nano Mater.*, 2020, **3**, 5665–5675.
- 101 5 V. Moreno, K. Murtada, M. Zougagh and Á. Ríos, *Spectrochim. Acta Part A Mol. Biomol.*
102 *Spectrosc.*, 2019, **223**, 117302.
- 103 6 F. Madzharova, Z. Heiner and J. Kneipp, *J. Phys. Chem. C*, 2020, **124**, 6233–6241.
- 104 7 S. Bonora, E. Benassi, A. Maris, V. Tugnoli, S. Ottani and M. Di Foggia, *J. Mol. Struct.*,
105 2013, **1040**, 139–148.
- 106 8 S. Dick and S. E. J. Bell, *Faraday Discuss.*, 2017, **205**, 517–536.
- 107 9 Y. Li, T. Gao, G. Xu, X. Xiang, X. Han, B. Zhao and X. Guo, *J. Phys. Chem. Lett.*, 2019,
108 **10**, 3013–3018.
- 109 10 A. J. Ruiz-Chica, M. A. Medina, F. Sánchez-Jiménez and F. J. Ramírez, *J. Raman*
110 *Spectrosc.*, 2004, **35**, 93–100.

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