Supporting Information

Highly-dispersed TiO₂ nanoparticles with abundant active sites induced by surfactant as a prominent substrate for SERS: Charge transfer contribution

Libin Yang,*a Di Yin,a Yu Shen, Ming Yang, Xiuling Li,a Xiaoxia Han,b

Xin Jiang*a and Bing Zhao*b

- a College of Pharmacy, Jiamusi University, Jiamusi 154007, People's Republic of China
- b State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun 130012, People's Republic of China
- * Corresponding authors. E-mail: ylb76@163.com (L.B. Y.); jiangxin@jmsu.edu.cn (X. J.); zhaob@mail.jlu.edu.cn (B. Z.)

Samples	BET/m ² ·g ⁻¹	$O_{V} O_{T}$
TiO ₂	123	0.84
6%P-TiO ₂	122	0.87
12%P-TiO ₂	120	0.94
18%P-TiO ₂	123	1.55
24%P-TiO ₂	120	1.38
30%P-TiO ₂	121	0.85
36%P-TiO ₂	124	0.83

Table S1 The BET surface area and XPS information of different TiO₂ NPs.

 $O_T:$ lattice oxygen, $O_V:$ vacancy oxygen; $O_V/O_T:$ the XPS peak area ratio of O_V and $O_T.$

Raman		SEDS	Assignment	
Solid	Solution	SERS	Assignment	
		1075w	benzene vibrations	
1122	1005	1135 w	The result of interaction between	
1132 VW	1132 vw 1095 w		the $\beta_{(NH2)}$ and $\beta_{(C-H)}$	
1180 w	1174 w	1179 w	Mixed vibration (benzene ring)	
1285 m	1268 w	1274 w	ν _(C-H) , ν _(O-H)	
1312 w	1339 w	1324 w	V _(C-C)	
		1403 w	$v_{C=O}$ (carboxyl group)	
1434 w	1452 w	1460 m	Mixed vibration (benzene ring)	
1601 w	1606 s	1602 s	Mixed vibration (benzene ring)	

Table S2 The Raman shifts and assignments of PABA molecule.

v: stretching vibration, β : rocking vibration; s: strong, m: medium, w: weak, vw: very weak.



Fig. S1 SAXRD patterns of as-prepared different TiO_2 samples.



Fig. S2 SERS spectra of 4-MBA adsorbed on the 18%P-TiO₂ (A) and TiO₂ (B) substrates from different concentration solution.