Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Simulation and synthesis of Fe_3O_4-Au satellite nanostructures for optimised surface-enhanced Raman scattering

The magnetic properties were measured by a vibrating sample magnetometer (VSM, LDJ9600, Troy, MI). The result indicated that the maximum saturation magnetization was 41 emu g^{-1} for FA satellite microspheres (Fig. S1). According to Ma's study, a saturation magnetization of 16.3 emu g^{-1} is sufficient for magnetic separation of particles from solution with a magnet.[1] The optical images were obtaining to further confirm the assemble of FA via applied magnetic field (inset of Fig. S1).

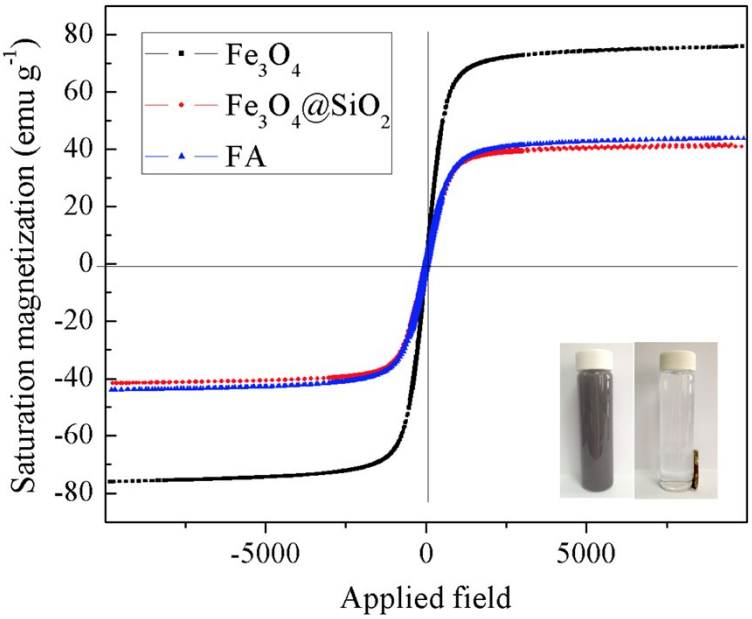

Fig. S1 Magnetic hysteresis loops of Fe_3O_4, Fe_3O_4@SiO_2, and FA. The inset illustrates the magnetic separation by an external magnet.

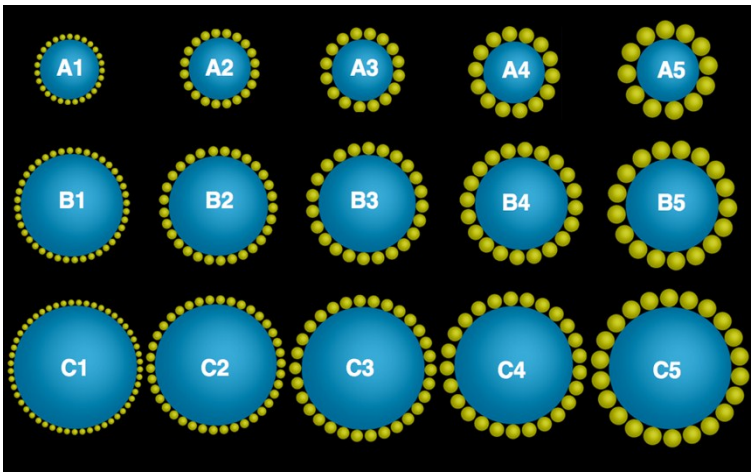

Fig. S2. FDTD models of Fe_3O_4-Au satellite system with Au NPs from 20 nm to 60 nm coated on 200 nm Fe_3O_4 (A1-A5), 300 nm Fe_3O_4 (B1-B5), and 400 nm Fe_3O_4 (C1-C5). The gap between Au NPs is 5 nm

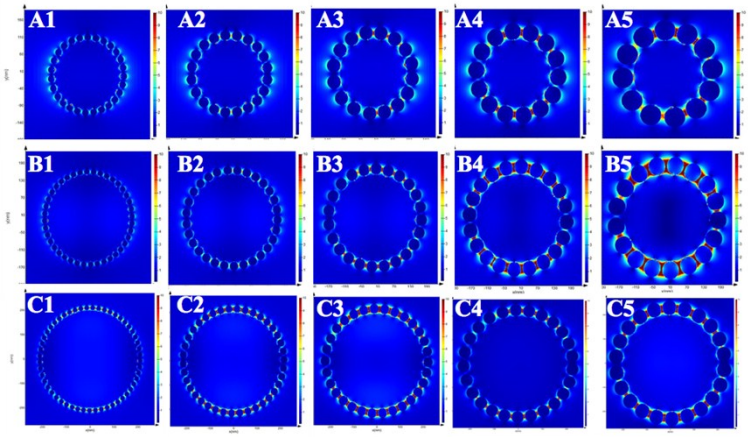

Fig. S3. EM distribution of satellite model with Au NPs from 20 nm to 60 nm coated on 200 nm Fe_3O_4 (A1-A5), 300 nm Fe_3O_4 (B1-B5), and 400 nm Fe_3O_4 (C1-C5). The gap between Au NPs is 5 nm.

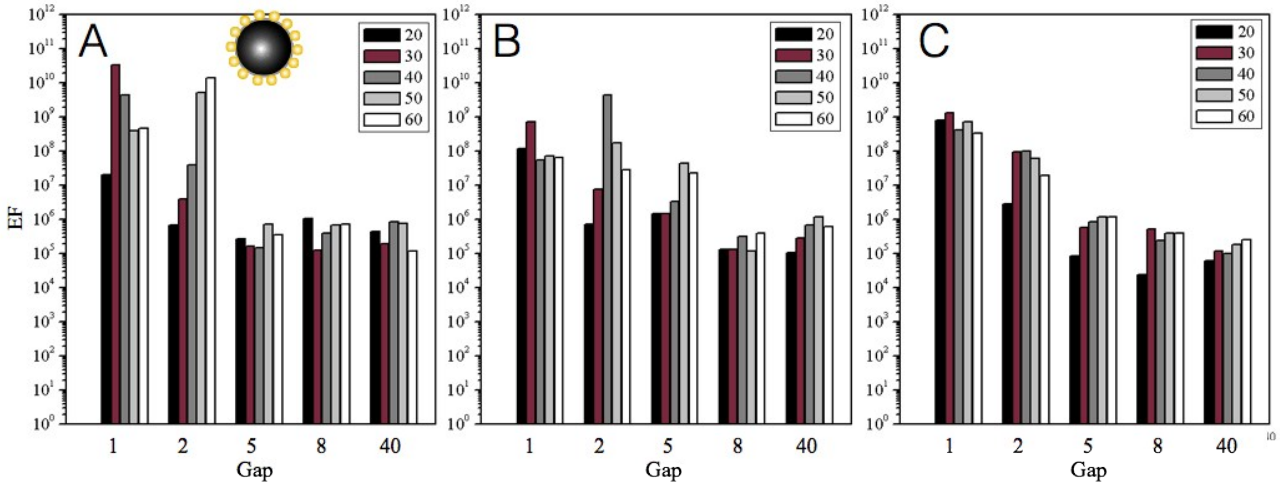

Fig. S4. The simulated SERS enhancement factors for magnetic satellite models with Fe_3O_4 size of 200 nm (A), 300nm (B) and 400 nm (C).

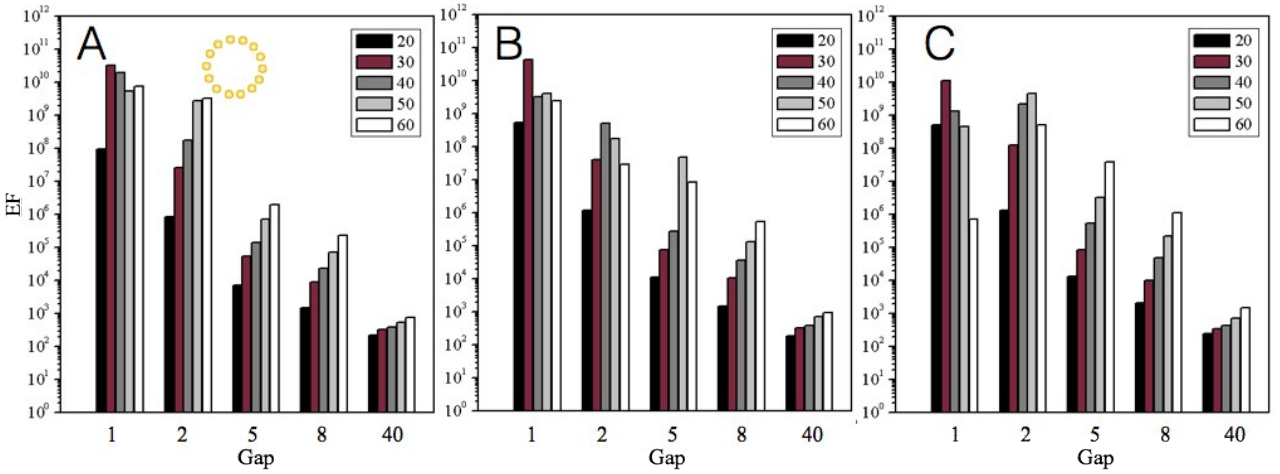

Fig. S5. The simulated SERS enhancement factors for hollow satellite models with core size of 200 nm (A), 300nm (B) and 400 nm (C).

Table S1. s/D values for FDTD models with Au NP size (*s,* 20 nm, 30 nm, 40 nm, 50 nm and 60 nm), and the gap distance between two adjacent Au NPs (D, 1 nm, 5 nm, 8 nm and 40 nm).

	20	30	40	50	60
1	20	30	40	50	60
2	10	15	20	25	30
5	4	6	8	10	12
8	2.5	3.75	5	6.25	7.5
40	0.5	0.75	1	1.25	1.5

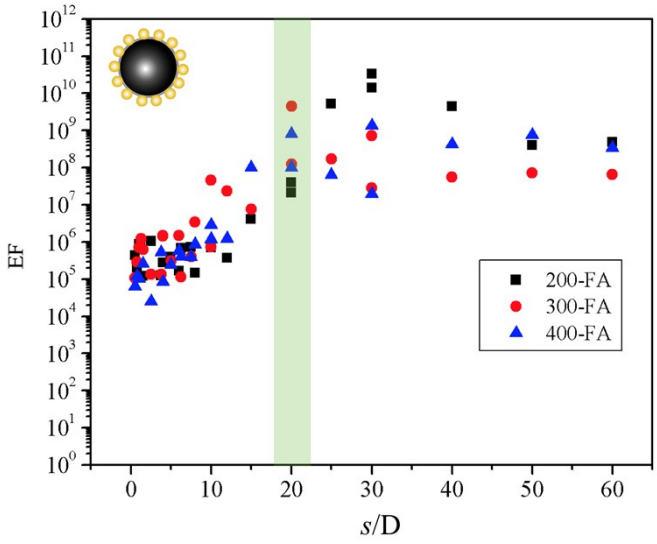

Fig. S6. The effect of size-to-gap ratio on the simulated enhancement factor for magnetic satellite system.

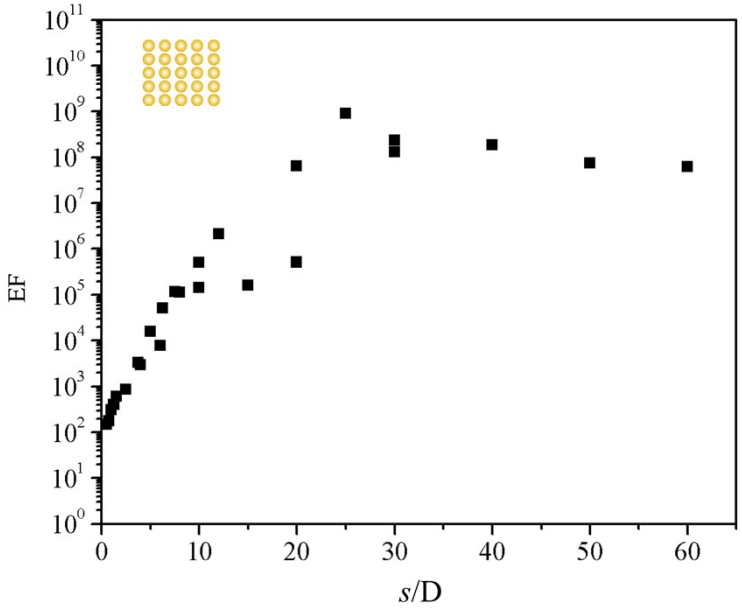

Fig. S7. The effect of size-to-gap ratio on the simulated enhancement factor for Au array system.

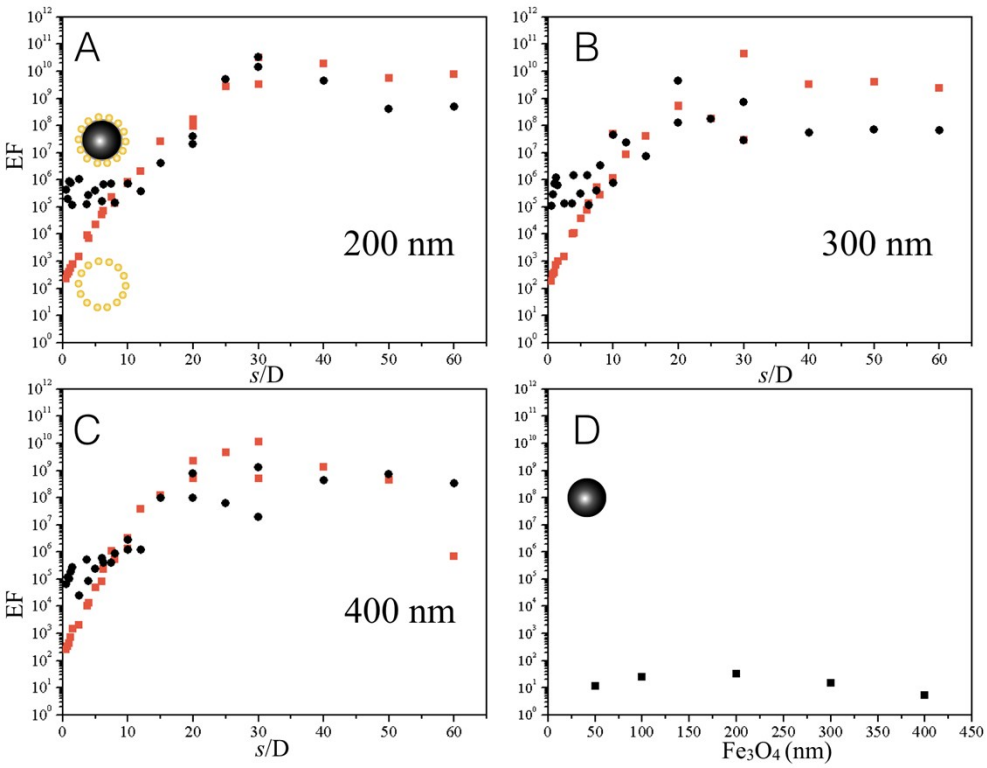

Fig. S8 The effect of size-to-gap ratio on the simulated enhancement factor for magnetic satellite system (red point) and hollow satellite system (black point) with core size of 200 nm (A), 300 nm (B) and 400 nm (C). (D) The effect of Fe_3O_4 diameter on the simulated enhancement factor.

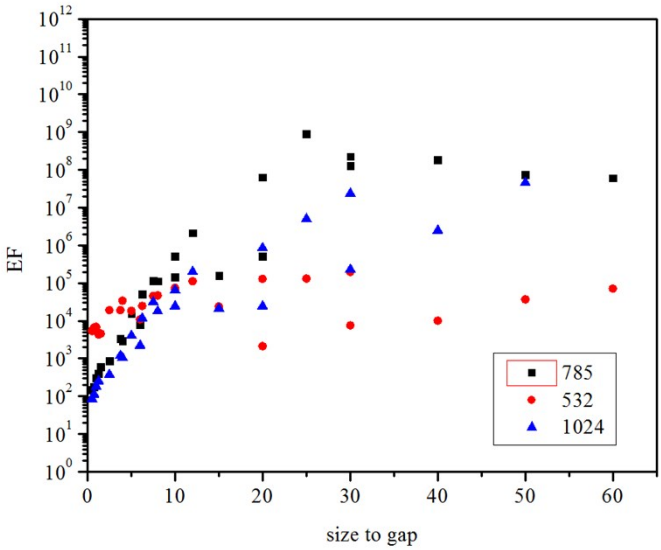

Fig. S9 The effect of size-to-gap distance ratio (*s*/D) on the simulated EF for array system at 532 nm, 785 nm and 1024 nm.

The selection of exciting wavelength

With an increase in the diameter of Au NPs from 21 to 57 nm, the corresponding UV-vis absorption peaks red-shifted from 520 to 548 nm (Fig. S10 A). Following the deposition of 20 nm Au NPs on 300 nm Fe_3O_4@SiO_2, the maximum absorption peak was red-shifted towards a higher wavelength (677 nm). This red-shift was attributed to the localized surface plasmon resonance of Au NPs (Fig. S10 B).[2] Therefore, when the diameter of Au NPs continued to increase from 21 to 57 nm, the UV absorption peak of the corresponding FA must be higher than 677 nm. Therefore, 785 nm was selected as the matched excitation wavelength.

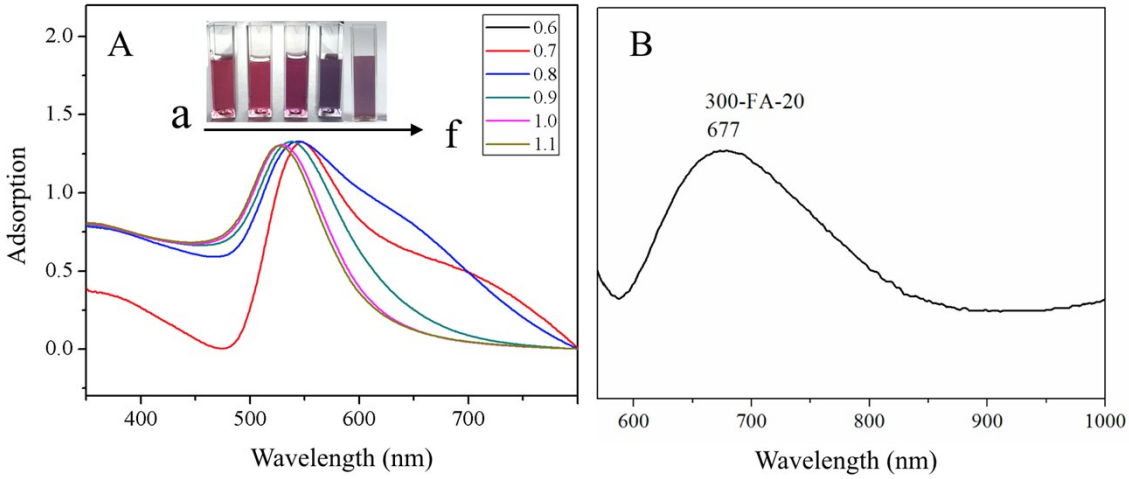

Fig. S10 (A) UV-vis spectra and color change of the synthesised Au NPs from 21 nm to 57 nm with citrate volume from 2 mL to 0.7 mL. (B) UV-vis spectrum of 300-FA-20.

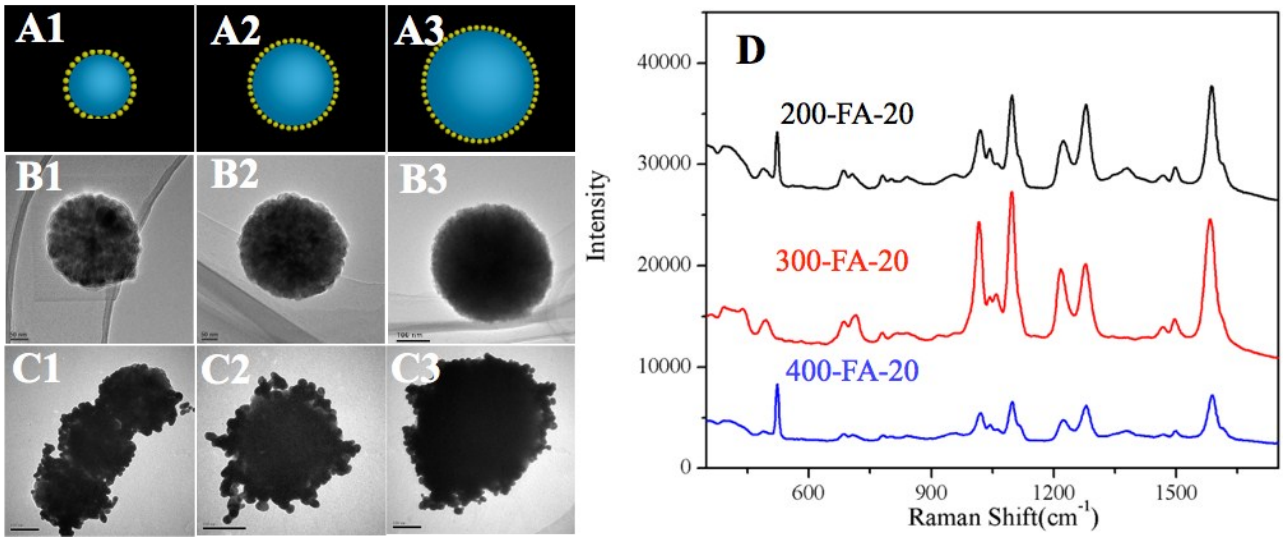

Fig. S11 FDTD (A1-A3), TEM image of Fe_3O_4@SiO_2 and TEM image of FA structure (B) with Au size of 20 nm, gap of 5 nm and Fe_3O_4 size of 200 nm (200-FA-20), 300 nm (300-FA-20) and 400 nm (400-FA-20). (D) SERS spectra of 1×10^{-5} M 4MPY(D) on substrate 200-FA-20, 300-FA-20 and 400-FA-20. Signal collecting time was 5 s.

Reference

1. Z. Ma, Y. Guan, H. Liu, *J. Polym. Sci., Part A: Polym. Chem.* **2005,** *43*, 3433.
2. L. Y. Wang, J. Luo, Q. Fan, M. Suzuki, I. S. Suzuki, M. H. Engelhard, Y. H. Lin, N. Kim, J. Q. Wang and C. J. Zhong, *J. Phys. Chem. B*, **2005**, **109**, 21593.