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Shape Controlled Synthesis of Concave Octahedral Au@AuAg Nanoparticles to Improved Their Surface-Enhanced Raman Scattering Performance

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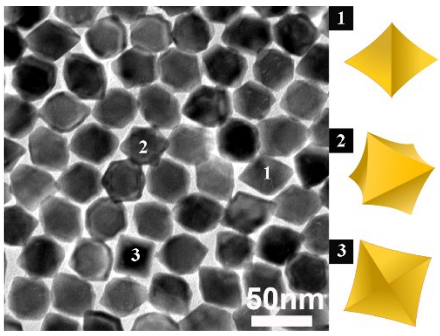

Fig. S1 a) TEM image of the as-synthesized concave octahedral Au@AuAg and the right panel show corresponding geometric models of a single NP orientated along different directions, respectively.

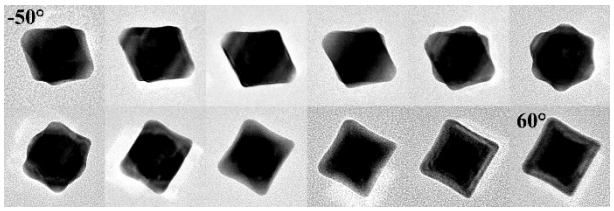

Fig. S2 A set of TEM images of an individual concaved octahedral Au@AuAg NP at different tilting angles with x as the axis of rotation from -50° to 60°.

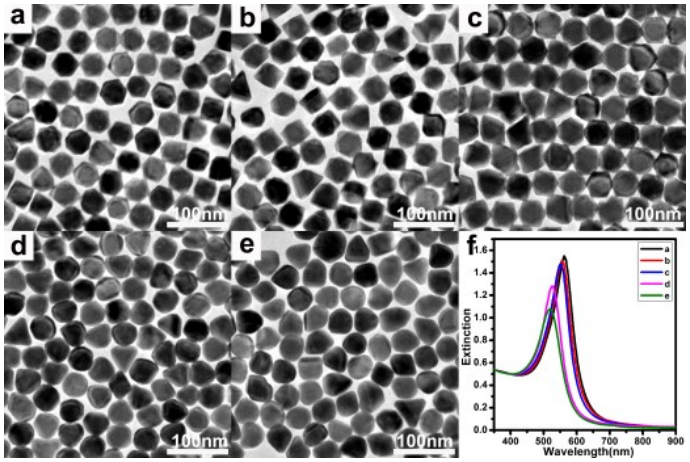

Fig. S3 TEM images (a to e) and UV-vis spectra (f) of Au NPs synthesized at different CTAC concentrations: 0.008 mM (a), 0.017 mM (b), 0.033 mM (c), 0.067 mM (d), and 0.133 mM (e). The volume of as-prepared short Au NRs solutions in the growth solution is 300 μL. The concentrations of CTAC, $AgNO_3$, $HAuCl_4$, and AA in the growth solution are 0.03 M, 100 μM, 0.24 mM, 1.44 mM, respectively.

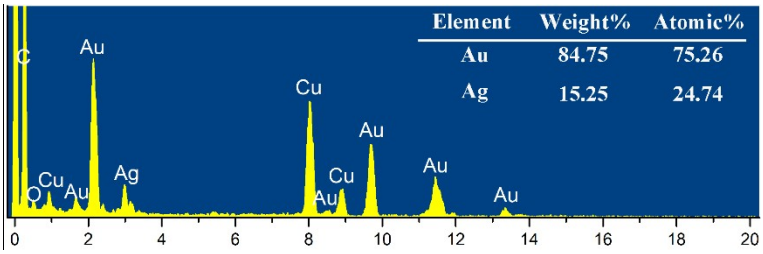

Fig. S4 Energy dispersive X-ray spectrometer (EDS) spectrum for Au@AuAg NPs on the copper grid. The atomic percentage of Au and Ag was 75.26 % and 24.74 %, respectively.

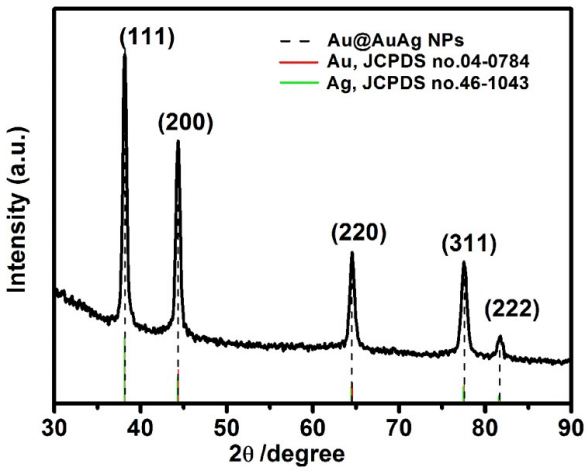

Fig. S5 XRD patterns of concave octahedral Au@AuAg NPs.

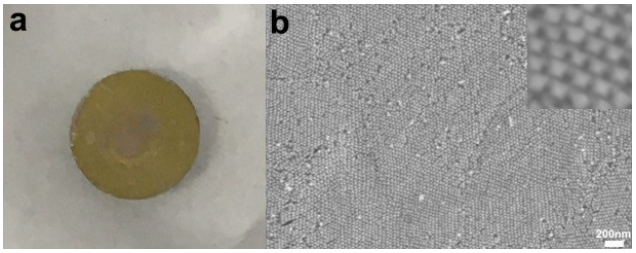

Fig. S6 Digital photos of the as-prepared self-assembled concave octahedral Au@AuAg NPs nano-film (a) and the corresponding SEM images of the self-assembled concave octahedral Au@AuAg NPs (b).

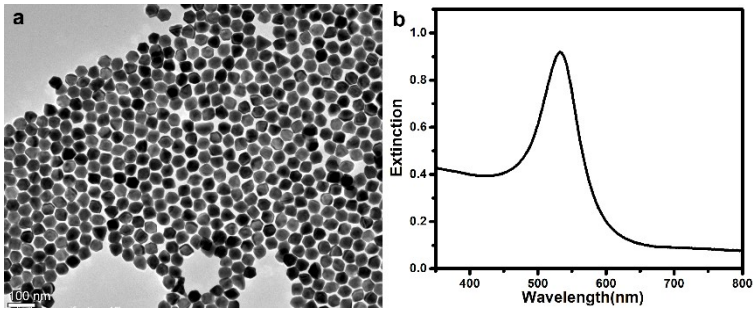

Fig. S7 TEM images (a) and UV-vis spectra (b) of octahedral Au NPs.

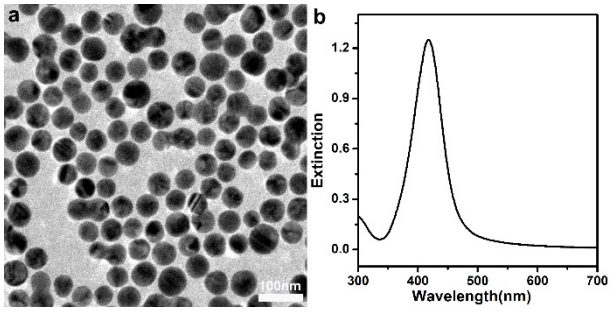

Fig. S8 TEM images (a) and UV-vis spectra (b) of Ag NPs.

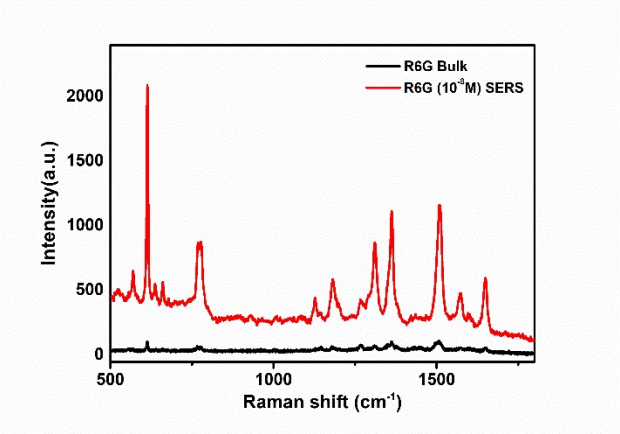

Fig. S9 The Raman spectra of R6G molecules on the blank glass substrate. The excitation laser wavelength for Raman measurements is 633 nm, the laser power is 0.2 mW, and the acquisition time is 10 s.

To quantitatively evaluate the SERS enhancement factor (EF) of the concave octahedral Au@AuAg NPs substrate, we employ the following equation[1,2]

$$EF = (I_{SERS} \times N_{Raman}) / (I_{Raman} \times N_{SERS})$$

where I_{SERS} and I_{Raman} represent the SERS and normal Raman intensities of the probe molecules acquired under identical conditions, including laser wavelength, laser power, acquisition time,– microscope objective, etc. N_{Raman} is the total number of probe molecules in the excitation volume for the normal Raman measurements and N_{SERS} is the total number of adsorbed molecules on the NPs in the SERS effective area. Fig. S8 show the Raman spectra of 10^{-2} M R6G from the as-prepared substrates. In this experiment, we select the intensity of the predominant peak of R6G at 613 cm^{-1} for the EF calculations.

TableS1. The atomic ratio of Au and Ag of the NPs synthesized at different $HAuCl_4$ concentrations: 0.083 (a), 0.167 (b), 0.24 (c), and 0.42 mM (d).

Sample no.	**a**	**b**	**c**	**d**
Au *w%*	74.25	81.4	84.8	89.1
Ag *w%*	25.75	18.6	15.2	11.9
Au:Ag (atomic ratio)	61.2/38.8	70.5/29.5	75.3/24.7	81.7/18.3

Table S2. The atomic ratio of Au and Ag of the NPs synthesized at different $AgNO_3$ concentrations: 33.3 μM (a), 66.7 μM (b), 100 μM (c), and 167 μM (d).

Sample no.	**a**	**b**	**c**	**d**
Au *w%*	93.8	89.3	80.5	74.8
Ag *w%*	6.2	10.7	19.5	25.2
Au:Ag (atomic ratio)	89.3/10.7	82.1/17.9	69.3/30.7	62.0/38.0

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2 A. N. Severyukhina, B. V. Parakhonskiy, E. S. Prikhozhdenko, D. A. Gorin, G. B. Sukhorukov, H. Möhwald, A. and M. Yashchenok, *ACS Appl. Mater. Interfaces* 2015, **7**, 15466–15473.