Supporting Information

Au@Ag Core-Shell Nanocubes with Finely Tuned and Well-Controlled Sizes, Shell Thicknesses, and Optical Properties

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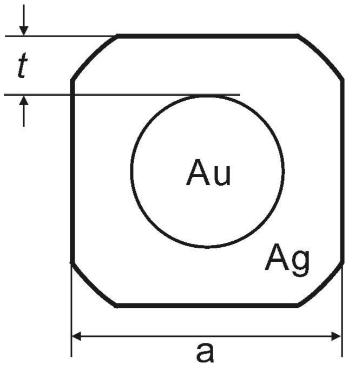
1. Definition of the Ag shell thickness:

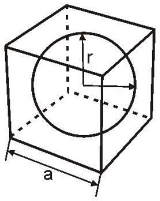


a: edge length of the Au@Ag nanocube,

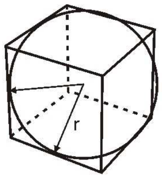
t: thickness of the Ag shell, calculated from:

$t = (a\text{-}d_{\text{core}})/2$, and d_{core}=11.0 nm for the CTAC-Au seeds.

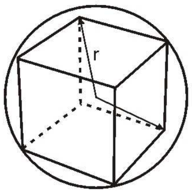
2. Radius (r) of virtual sphere used in the description of truncation:



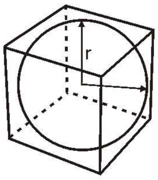
r=a/2



r=1.41a/2



r=1.73a/2



r=1.25a/2

When a model of a spherical Au core and cubic Ag shell (without truncation) was used, we found that the extinction peak position around 500 nm stayed almost unchanged when the thickness increased, showing discrepancy with the experimental data. Considering the possible slight truncation for the cubic structure, we modified the model to a spherical Au core and cubic Ag shell with a certain degree of truncation at corners. We used a virtual sphere of radius r to describe such a truncation. When $r=a/2$ (where a is the edge length of the cube), the sphere touches the 6 faces of the cube; when $r=1.41(a/2)$, the sphere touches the 12 edges of the cube; when $r= 1.73(a/2)$, the sphere touches the 8 corners of the cube. For $r=1.25(a/2)$, the UV-vis spectra for different Ag shell thicknesses agreed well with the experimental data (see Figure 6).

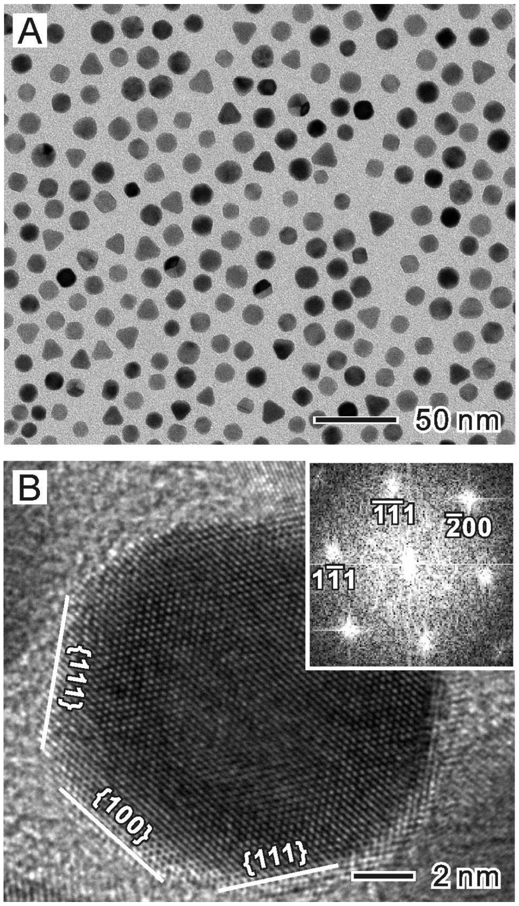


Figure S1. (A) TEM image of Au seeds (13.8±1.2 nm) prepared using the same two-step method except the use of CTAB as a capping agent. (B) High-resolution TEM image of a representative, CTAB-covered Au seed, which was an octahedron with slight truncation at corners.

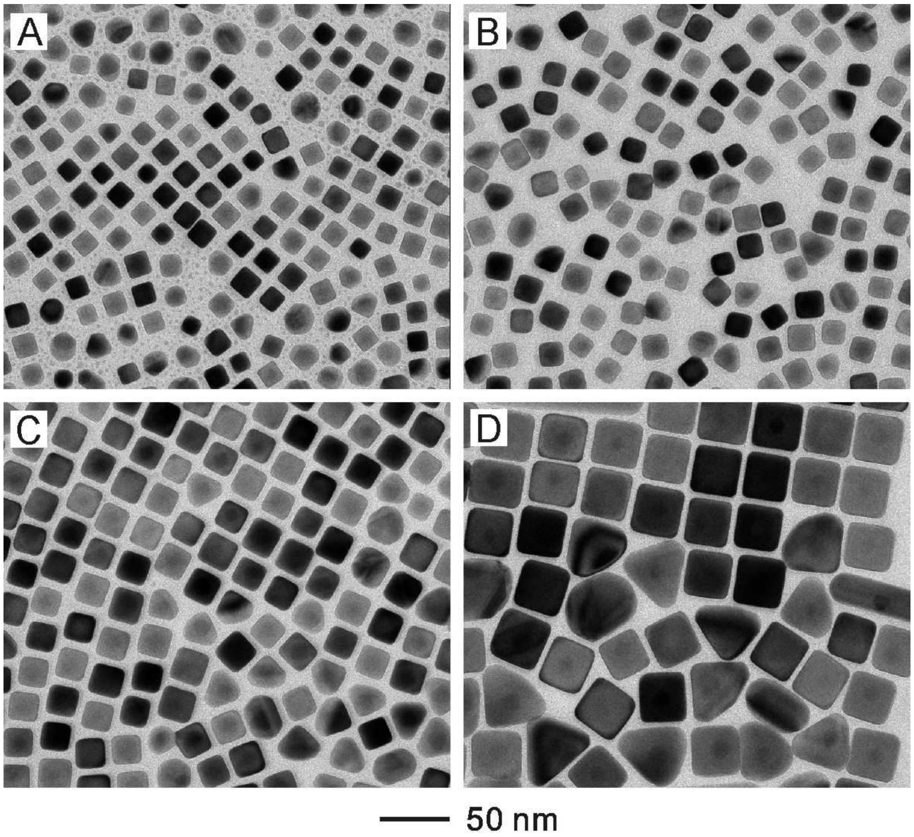


Figure S2. TEM images of Au@Ag nanocubes prepared under the same conditions as in Figure 2, except the use of Au seeds covered by CTAB instead of CTAC. After the addition of $AgNO_3$ and AA, the final concentrations of $AgNO_3$ were: (A) 0.09, (B) 0.17, (C) 0.29, and (D) 0.67 mM, respectively.

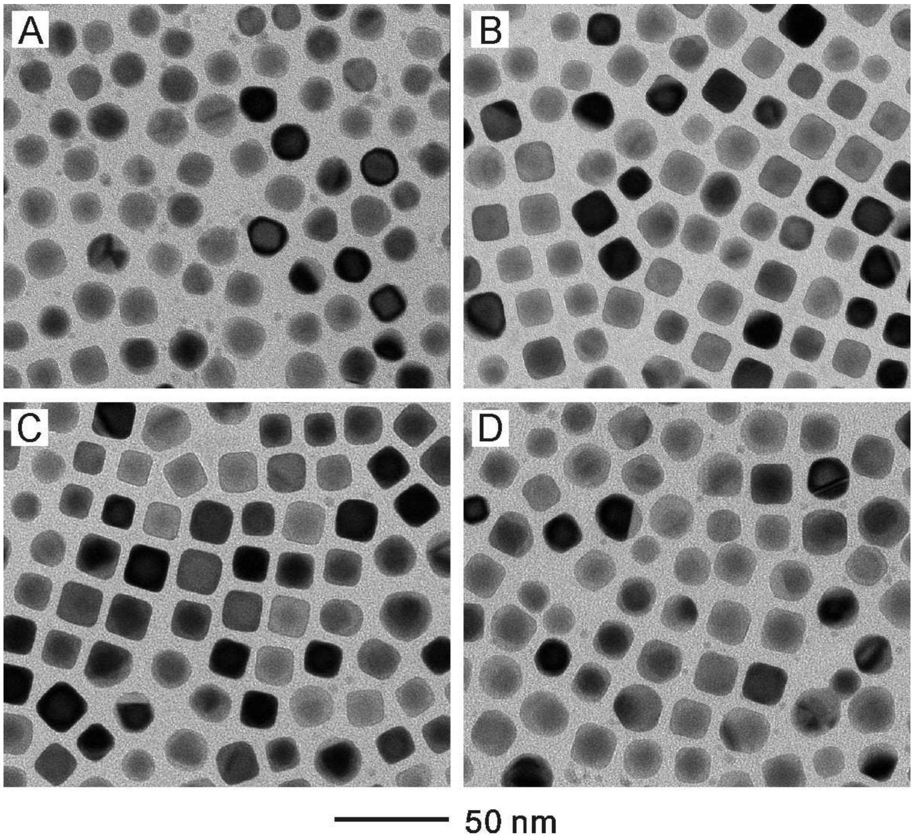


Figure S3. TEM images of the samples obtained under the same conditions as in Figure 4, except for the use of Au seeds covered by CTAB instead of CTAC. After the addition of $AgNO_3$ and AA, the concentrations of $AgNO_3$ were: (A) 0.09 mM, (B) 0.17 mM, (C) 0.29 mM, and (D) 0.67 mM, respectively.

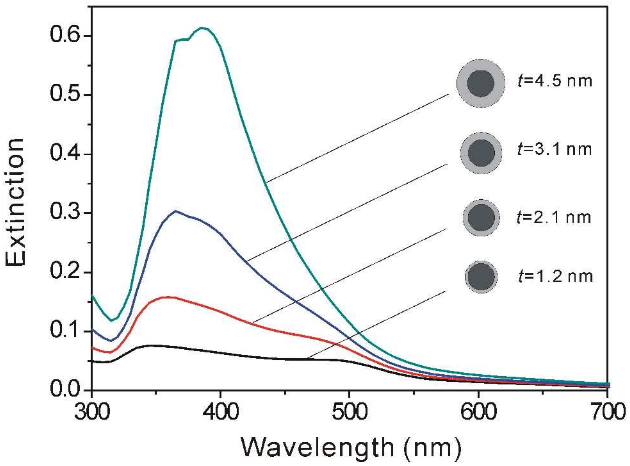


Figure S4. Extinction spectra calculated for Au@Ag nanospheres using Mie theory.

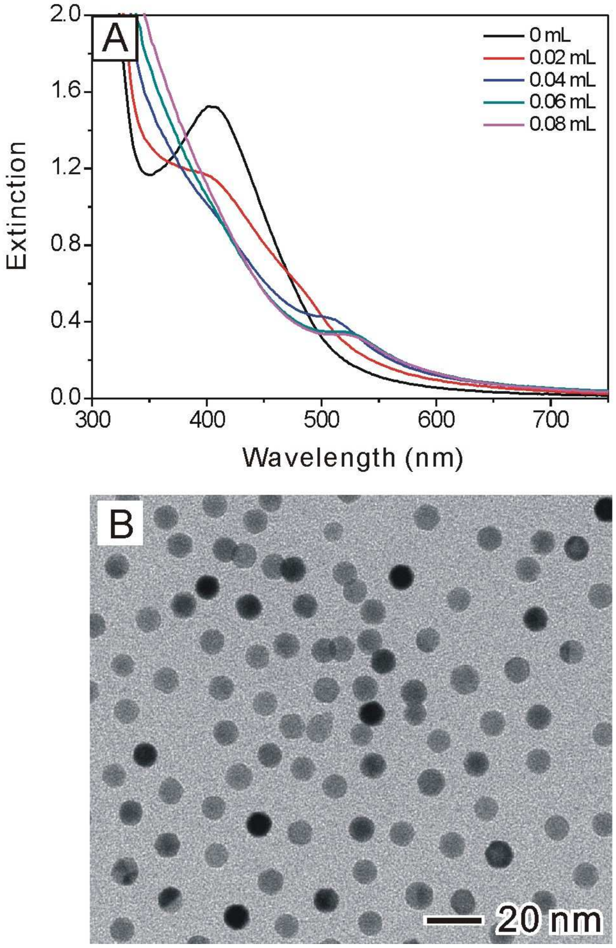


Figure S5. (A) Extinction spectra of the products obtained by dissolving Au@Ag core-shell nanocubes (17.2 nm, *t* =3.1 nm) with 0.05 M of $Fe(NO_3)_3$ solution. The main LSPR peak shifted from Ag (around 410 nm) to Au (around 524 nm) when the volume of $Fe(NO_3)_3$ solution was increased from 0 to 0.08 mL. When 0.06 mL of $Fe(NO_3)_3$ solution was added, the LSPR peak of Ag shells disappeared, and only the peak for the Au cores remained. (B) TEM image of the Au cores obtained by dissolving Au@Ag core-shell nanocubes with 0.08 mL of $Fe(NO_3)_3$ solution.