Supporting Information

Facile Synthesis and Heteroepitaxial Growth Mechanism of Au@Cu Core-Shell Bimetallic Nanocubes Probed by First-Principles Studies

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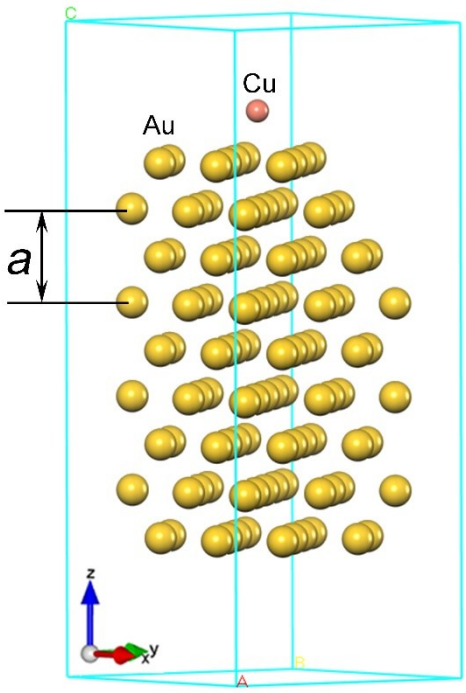

Figure S1. Supercell for Au/Cu configuration in ball-stick format. Yellow and red balls represent Au and Cu atoms respectively. The *z*-axis is perpendicular to the *xy*-plane, *a* is the lengths of one crystal cell in *z*-direction, named as lattice constant.

Au and Cu Lattice Constants with DFT

The bulk Au and Cu lattice constants a were calculated using a face-centered cubic (*fcc*) primitive cell. For calculation of Au lattice constant, the cell built with different lattice constants ranging between 4.09 and 4.28 Å with the step of 0.01 Å. We used a (10× 10× 10) k-point grid for this primitive cell. We plotted the energy and the lattice constant and found 4.18 Å at the location where the corresponding bulk Au cohesive energy is $E_{\text{bulk-Au}}$ = -3.247 eV. For calculation of Cu lattice constant, the cell built with different lattice constants ranging between 3.55 and 3.73 Å with the step of 0.01 Å. We also used a (10× 10× 10) k-point grid for this primitive cell. We plotted the energy and the lattice constant and found 3.64 Å at the location where the corresponding bulk Cu cohesive energy is $E_{\text{bulk-Cu}}$ = -3.704 eV. These values are in exact agreement with previous PBE theoretical results.

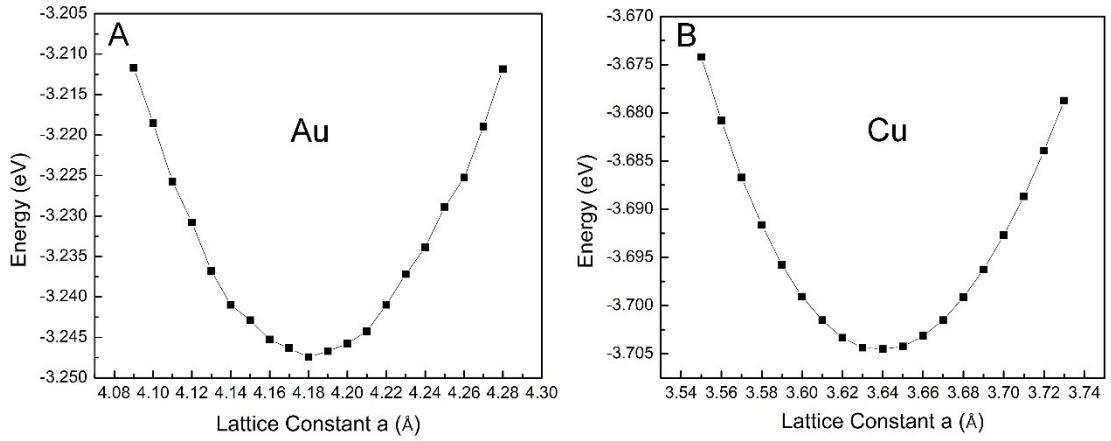

Figure S2. Calculation of bulk energy corresponding to different lattice constants: (A) for Au, (B) for Cu.

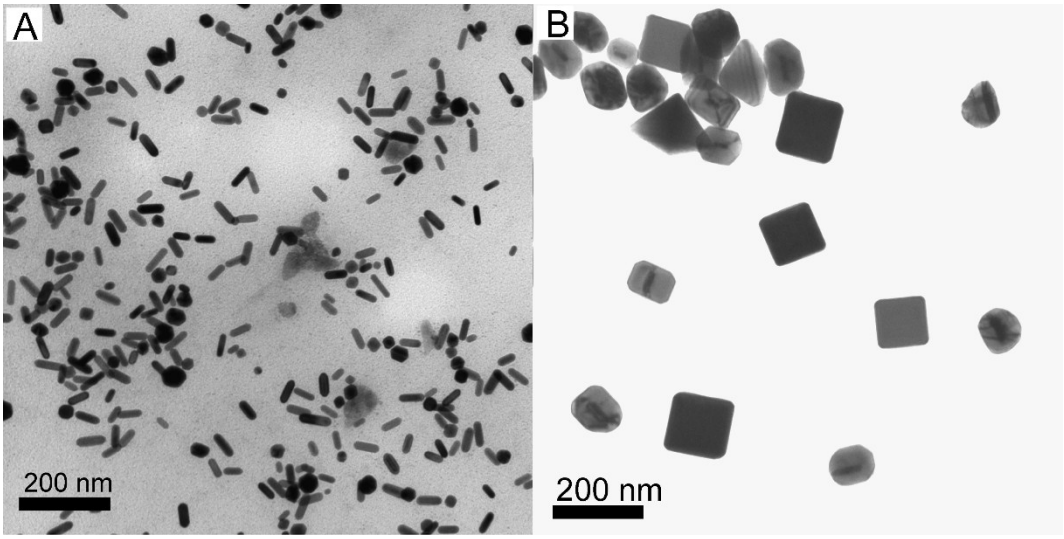

Figure S3. TEM images of the as-obtained Au@Cu nanocrystals prepared at different amounts for the Cu precursor: (A) 10 mg, (B) 34 mg.

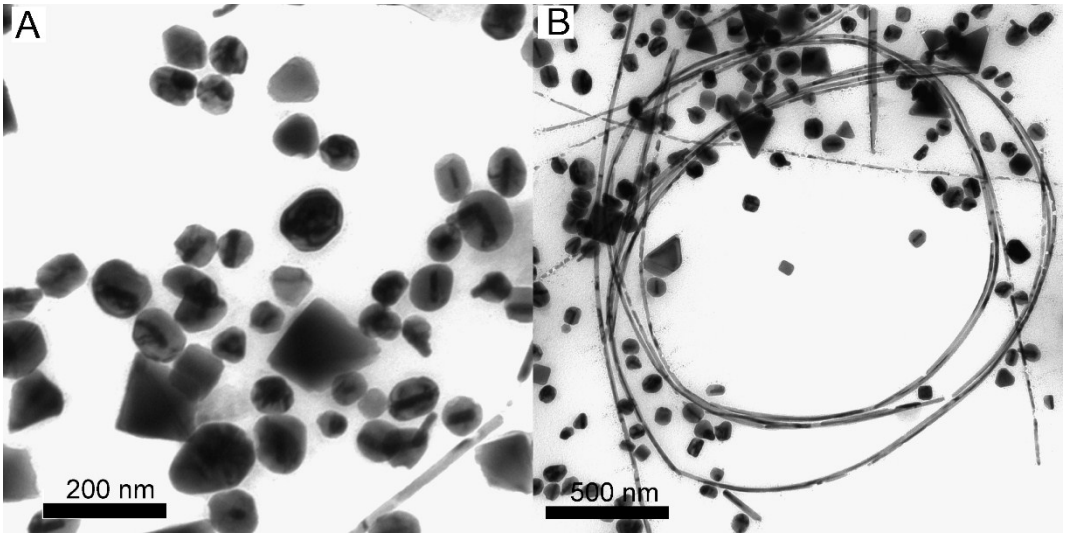

Figure S4. TEM images of the as-obtained Au@Cu nanocrystals prepared at different amounts for the HDA: (A) 60 mg, (B) 180 mg.

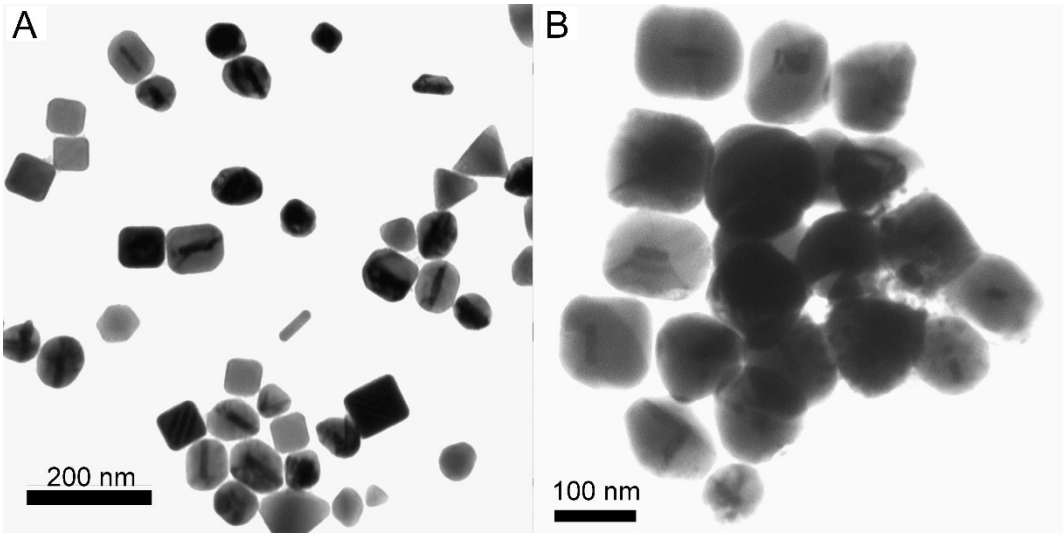

Figure S5. TEM images of the as-obtained Au@Cu nanocrystals prepared at different amounts for the glucose: (A) 30 mg, (B) 90 mg.