Synthesis of Tetrahexahedral Au Nanocrystals with Exposed High-Index Surfaces

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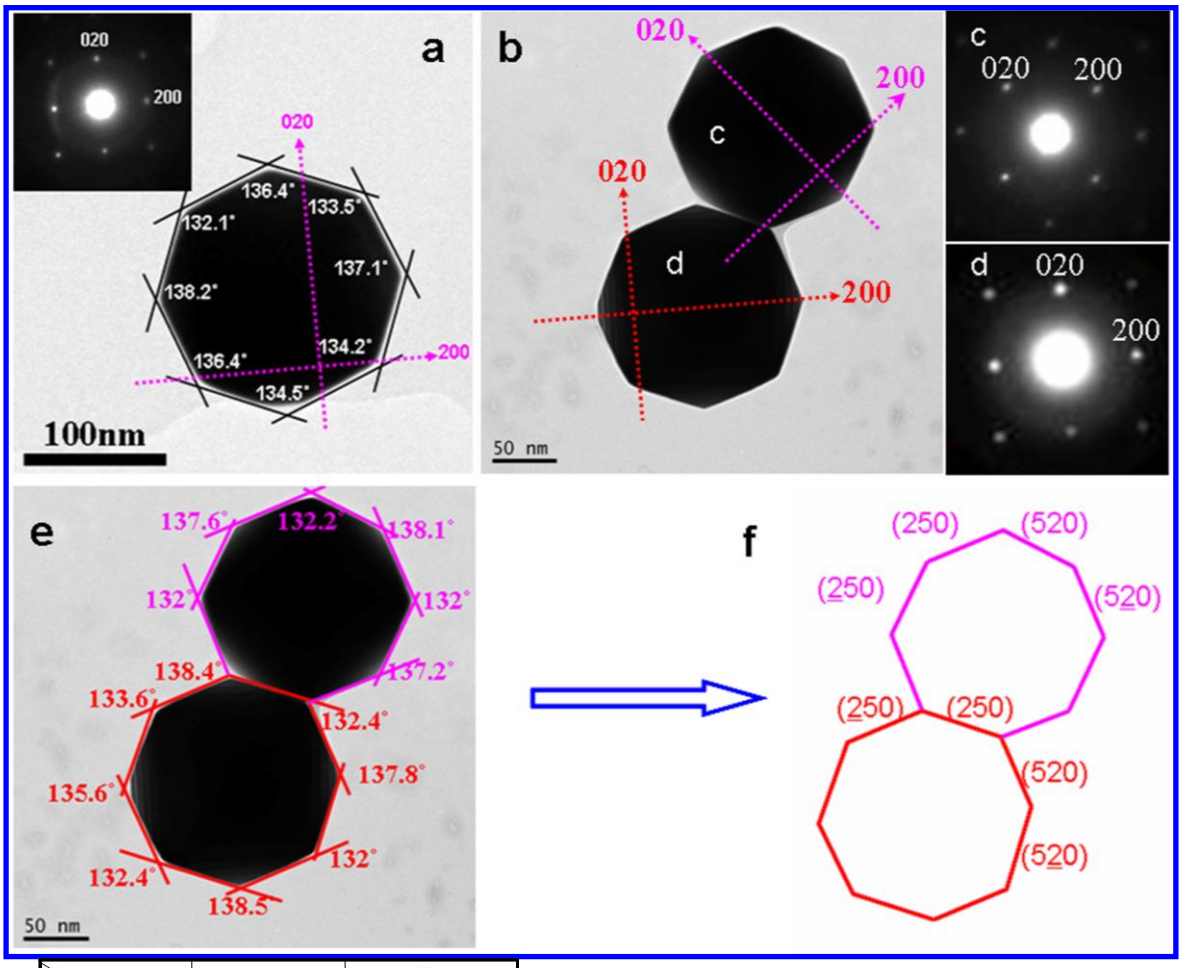

Angle / {hkl}	α	β
{210}	126.87°	143.13 °
{520}	**136.40 °**	**133.60°**
{730}	133.60 °	136.40°
{310}	143.13 °	126.87 °

Fig. S1 Determining the facets of the THH Au NCs. (a) TEM image of a THH and its interfacial angles. (b) TEM image of another two THH particles and corresponding SAED patterns (c, d). The exposed facets of the THH can be identified by a conjunction analysis of the angles between the facets, the TEM image and the SAED patterns of the Au particles, as shown in (e) and (f). The result indicates that the THH Au NCs are enclosed by {520} facets. The table shows the theoretical interfacial angles of different facets.

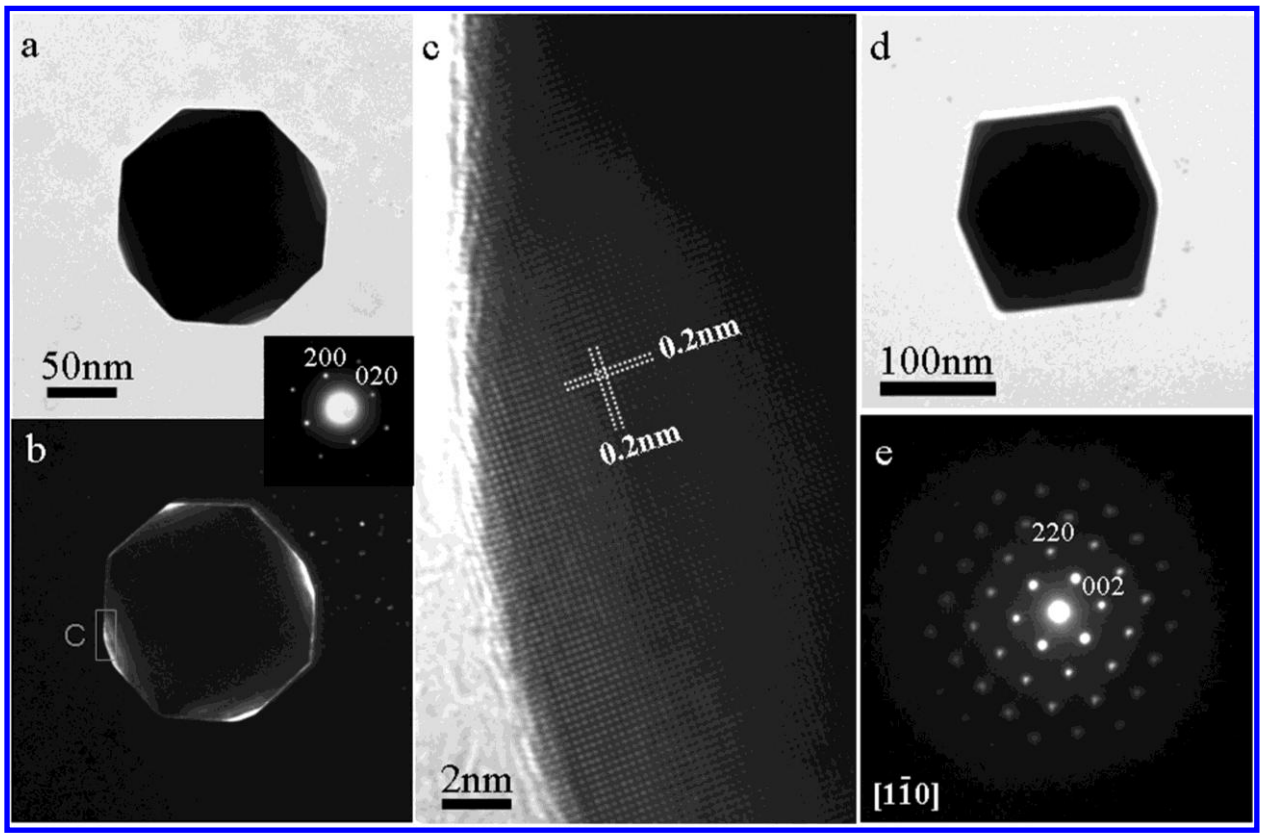

Fig. S2 (a) Bright-field and (b) Dark-field TEM image of a THH Au nanoparticle oriented along [001] direction, the SAED patterns shown as inset. (c) High-resolution TEM image from the region boxed in (b). (d) TEM image of a THH Au nanoparticle viewed along [1$\underline{1}$0] direction and (e) the corresponding electron diffraction pattern.

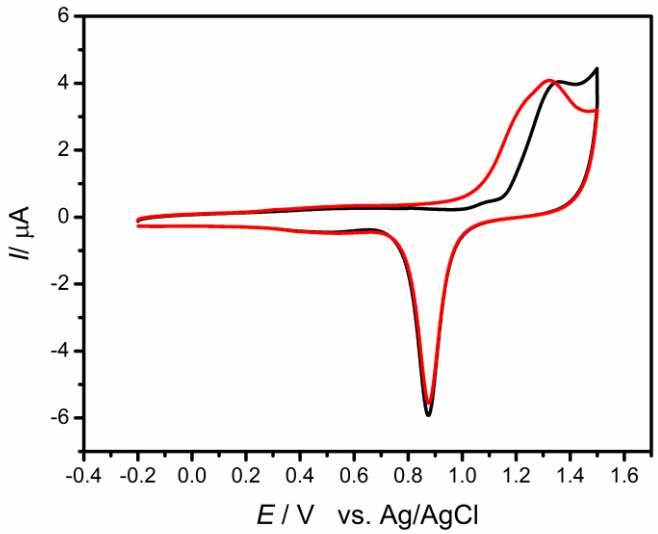

Fig. S3 Cyclic voltammograms of bulk Au (111) single-crystal electrode in 0.5 M H_2SO_4 in absence (black) and presence (red) of 1 M formic acid at the scan rate of 50 mV/s.

Experimental procedure of characterization of electrocatalytic activity: Electrochemical measurements were performed with a CHI 660C Electrochemical Analyzer (CH instrument, USA) in a conventional three-electrode cell. THH Au NCs modified glassy carbon electrode (THH-Au-NCs/GCE) or a bulk Au (111) single-crystal electrode was used as the working electrode, a platinum wire as the counter electrode and an aqueous Ag/AgCl as the reference electrode. A GCE was polished with 1.0, 0.3, and 0.05 μm alumina slurry sequentially and then washed ultrasonically in water and then ethanol for a few minutes. The cleaned electrode was modified with 10 μL homogeneous suspension of 5 mL/mg THH-Au-NCs in water, and then was dried overnight. 0.5 M H_2SO_4 solution was deaerated by pure nitrogen bubbling prior to CV measurements and the electrochemical cell was kept under a nitrogen atmosphere throughout the experiments. Formic acid was added into the 0.5 M H_2SO_4 solution using a microliter syringe.

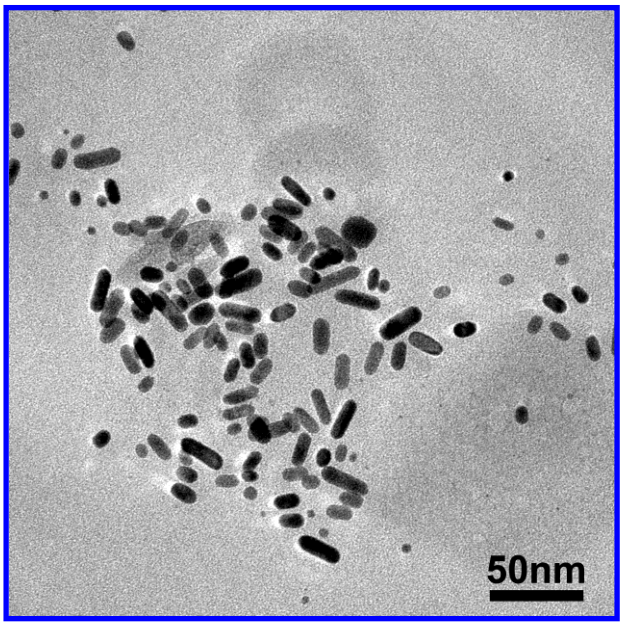

Fig. S4 TEM image of the product fabricated by using CTAB (0.005 M, 5 mL) instead of DDAB (0.005 M, 5 mL) in the synthesis of quasi-THH Au NCs while keeping other experimental conditions the same.

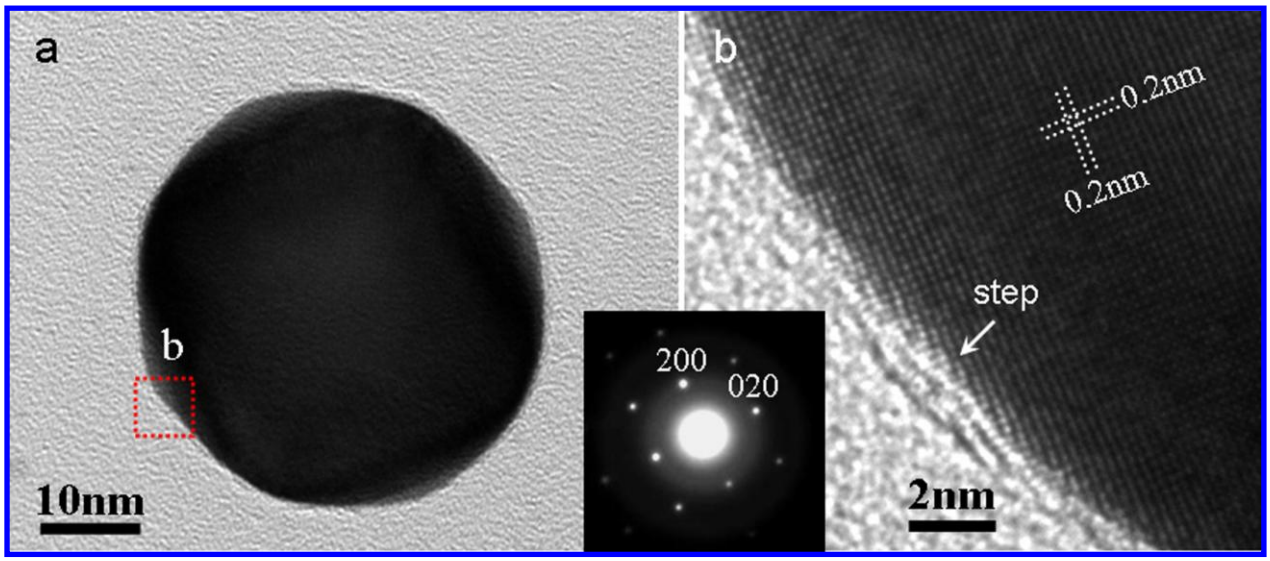

Fig. S5 (a) TEM image of single quasi-THH Au nanoparticle oriented along [001] direction and (b) the HRTEM recorded from boxed region marked in (a).

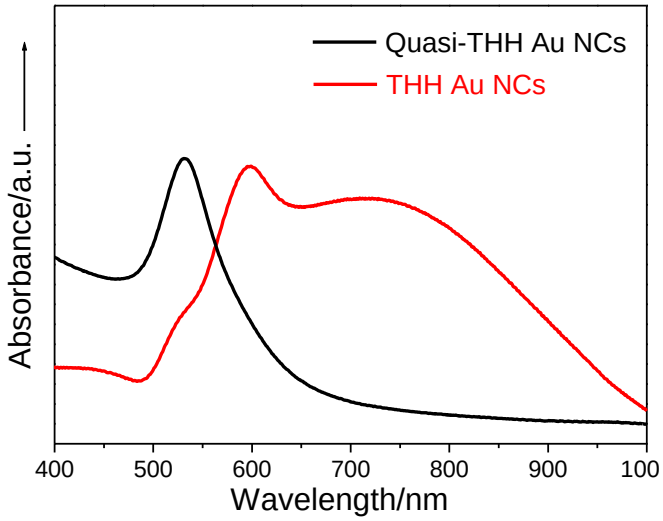

Fig. S6 Ultraviolet-visible (UV-vis) absorption spectra of the quasi-THH and THH Au NCs solution.