Electronic Supplementary Information

{331}-Faceted Trisoctahedral Gold Nanocrystals: Synthesis, Superior Electrocatalytic Performance and High Efficient SERS Activity

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Figure S1. TEM images (a and b) and Extinction spectra (c) of the corresponding TOH Au NCs obtained with CTAB-Au seeds (a, black curve) and CTAC-Au seeds (b, red curve), respectively. The volumes of the Au seeds solution used both are 0.125 μL. The concentrations of CTAC, $HAuCl_4$, and AA in the reaction mixture are 47, 0.47, and 0.94 mM, respectively.

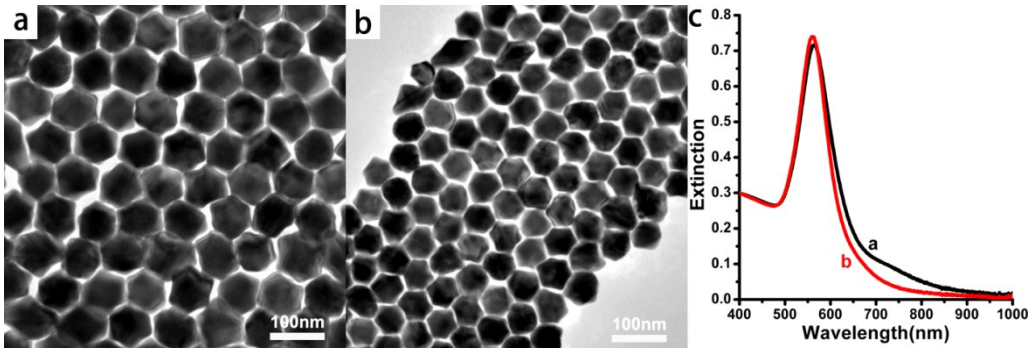

Figure S2. TEM images (a and b) and Extinction spectra (c) of the corresponding TOH Au NCs obtained with CTAB-Au seeds (a, black curve) and CTAC-Au seeds (b, red curve), respectively. The volumes of the Au seeds solution used both are 0.075 μL. The concentrations of CTAC, $HAuCl_4$, and AA in the reaction mixture are 47, 0.47, and 0.94 mM, respectively.

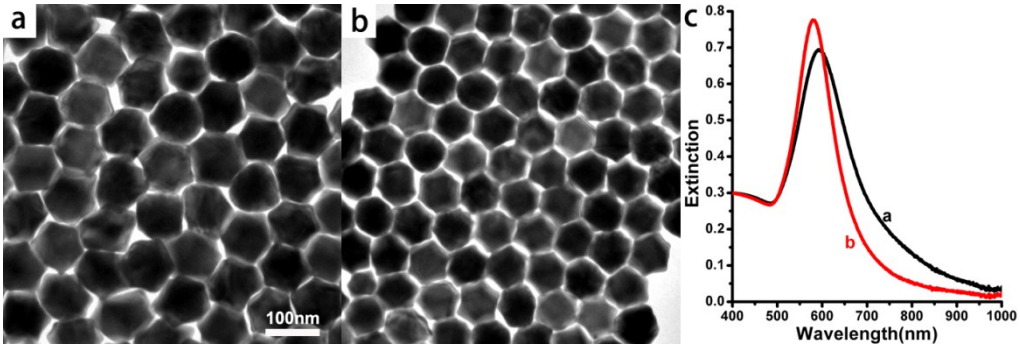

Figure S3. Cyclic voltammograms (CVs) of the corresponding TOH Au NCs with {221} facets (black curve) and {331} facets (red curve) in 0.50 M H_2SO_4 media. The currents are normalized by the Au mass loaded. The scan rate is 50 mV s^{-1}. The TOH Au NCs are obtained with CTAB-Au seeds (black curve) and CTAC-Au seeds (red curve). The volume of the Au seeds solution used both are 0.05μL. The concentrations of CTAC, $HAuCl_4$, and AA in the reaction mixture are 47, 0.47, and 0.94 mM, respectively.

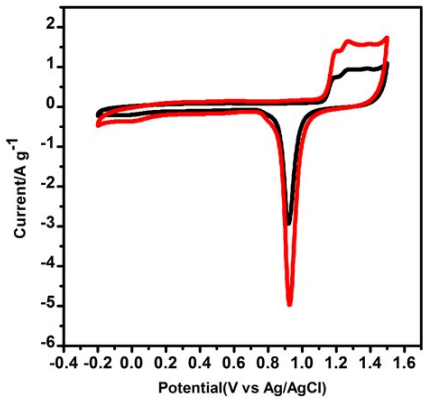

Figure S4. Cyclic voltammograms (CVs) of TOH Au NCs with different sizes in 0.50 M H_2SO_4 media. The currents are normalized by the Au mass loaded on the electrodes. The scan rate is 50 mV s^{-1}. The sizes of TOH Au NCs are indicated as the different colored curves.

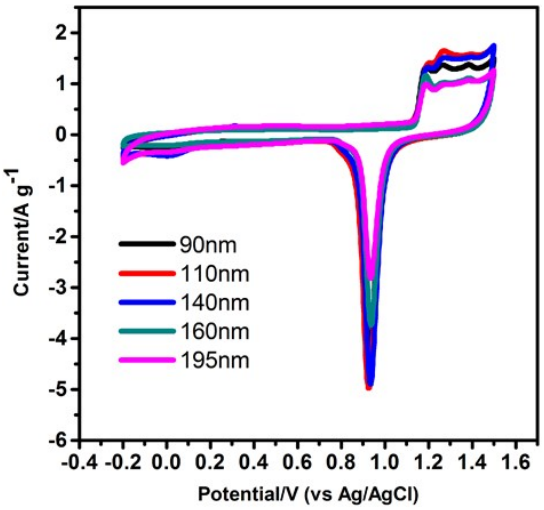

Figure S5. Cyclic voltammograms (CVs) of TOH Au NCs with different sizes in 0.50 M KOH media normalized by Au mass loaded on the electrodes (a), in 0.50 M KOH media containing 1.0 M methanol normalized by Au mass loaded on the electrodes (b), and in 0.50 M KOH containing 1.0 M methanol normalized by their ECSAs (c). The peak areas are associated with the reduction of Au oxide species and are used for the evaluation of the ECSAs. The scan rate is 20 mV s^{-1}. The sizes of TOH Au NCs are indicated as the different colored curves.

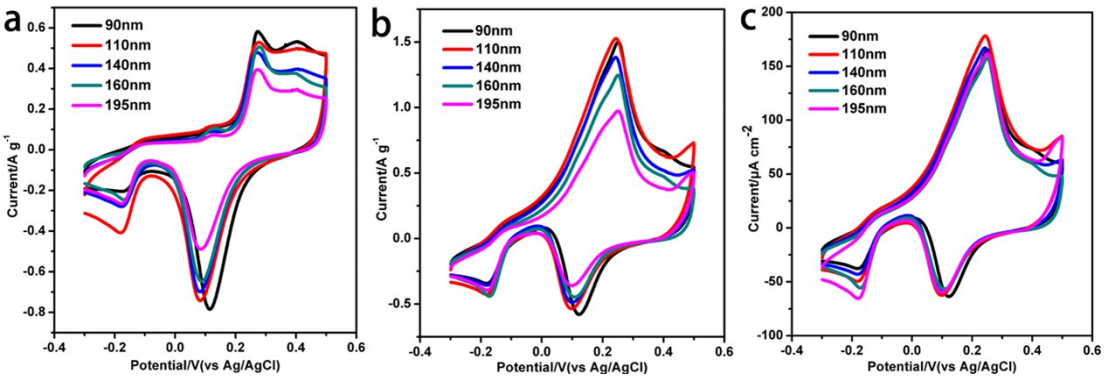

Figure S6. The variation of oxidation peak current density of the GCEs modified by the 110 nm TOH Au NCs at different scanning cycle numbers. The CV curves are recorded in 0.50 M KOH media containing 1.0 M methanol. The scan rate is 20 mV s^{-1}.

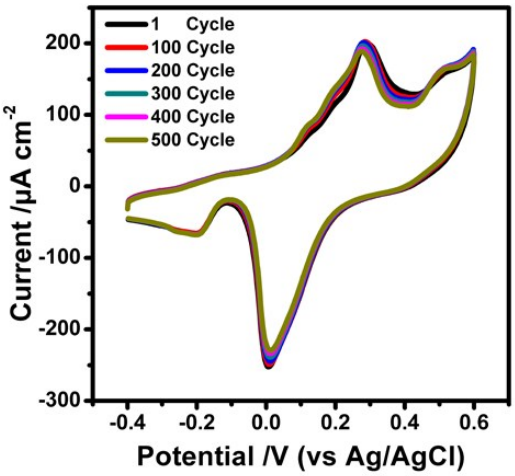

Figure S7. Experimental extinction spectra of TOH Au NCs of different sizes on glass substrates.

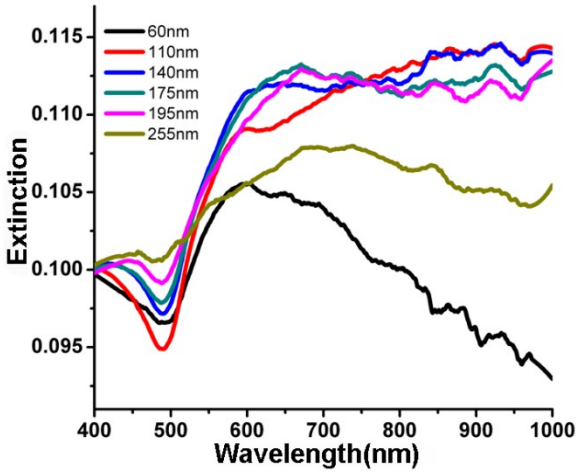

Figure S8. SERS spectra of 4-ATP molecules (3×10^{-4} M) on the aggregates of 175 nm TOH Au NCs (i) and 170 nm spherical Au NCs (ii), respectively. The excitation laser wavelength for Raman measurements is 633 nm. The acquisition time is 10 s.

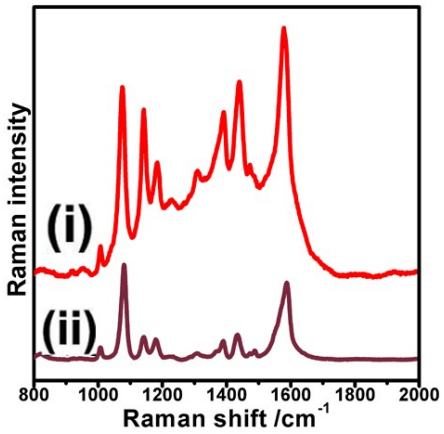

Figure S9. Normal Raman spectrum of the neat film of 4-ATP molecule. The acquisition time was 10 s.

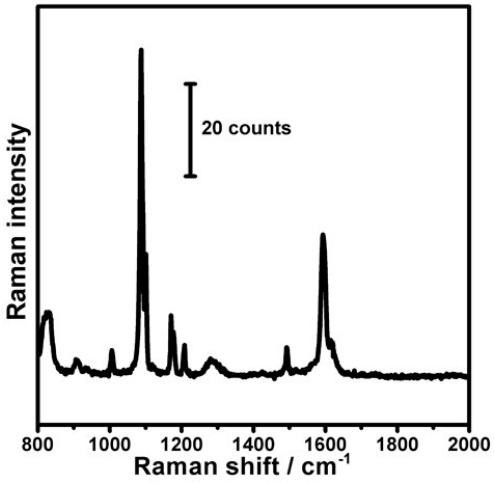

Table S1. Summarized data of the Raman intensity and SERS enhancement factors (EFs) of 4-ATP molecules of the TOH Au NCs of different sizes in specific Raman bands.

Size/nm	I_{1080}	EF_{1080}	I_{1578}	EF_{1578}
60	23705	1.05×10^7	18212	1.83×10^7
110	38313	1.69×10^7	45822	4.60×10^7
140	53069	2.34×10^7	67648	6.78×10^7
175	77386	3.42×10^7	112868	1.13×10^8
195	72419	3.20×10^7	68836	6.90×10^7
255	51315	2.26×10^7	50101	5.00×10^7

Table S2. Summarized data of the electrooxidation of methanol catalyzed by the TOH Au NCs of different sizes.

Size [nm]	ECSA [$m^2\ g^{-1}$]	Potential [V]	Mass activity [$A\ g^{-1}$]	Specific activity [$mA\ cm^{-2}$]
90	0.909	0.252	1.50	0.165
110	0.857	0.244	1.53	0.178
140	0.828	0.244	1.38	0.167
160	0.791	0.250	1.25	0.162
195	0.602	0.251	0.970	0.158