Rational design and synthesis of excavated Au nanocrystals

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**Figure S1.** a) SEM image of the as-synthesized TOH Au NCs; b) Enlarged SEM images of TOH Au NCs viewing from different directions and their corresponding models, which are bounded by 24 \{221\} facets.

**Figure S2.** SEM images of corresponding Au-Pd heterogeneous NCs synthesized by varying the amount of aqueous solution of H$_2$PdCl$_4$ (1.0 mmol L$^{-1}$): a) 0.10 mL, b) 0.30 mL, c) 0.50 mL, d) 0.70 mL, e) 1.0 mL, f) 3.0 mL, respectively.
**Figure S3.** SEM images of Au NCs synthesized at different temperatures: a) 6 °C, b) 30 °C, c) 50 °C. The amount of aqueous solution of HAuCl$_4$ (1.0 mmol L$^{-1}$) was 3.0 mL.

**Figure S4.** XRD pattern of the excavated TOH Au NCs.

**Figure S5.** SEM images, high-magnification TEM images, corresponding SAED patterns and schematic models of an individual excavated TOH Au NCs viewed along [001] and [013] directions, respectively.
Figure S6. Schematic model for the growth orientation of the excavated TOH Au nanocrystal.

Figure S7. a) CV curve of the excavated TOH Au NCs loaded onto a glassy carbon electrode; b) CV curve of a polycrystalline gold electrode. (Tested in 0.1 M H₂SO₄ at the scan rate of 50 mV s⁻¹)
Figure S8. SEM images of the Au NCs synthesized in refrigerator: a) original temperature of reaction solution is 30 °C; b) original temperature of reaction solution is 12 °C.

Figure S9. EDS of the as-synthesized excavated TOH Au-Pd alloy NCs.
Figure S10. a) SEM image of the TOH Au NCs with the same size of the excavated TOH Au NCs; b) Enlarged SEM images of TOH Au NCs viewing from different directions and their corresponding models, which are bounded by 24 \{221\} facets.

Figure 11. The comparison of extinction spectra of TOH Au NCs (black line) and excavated TOH Au NCs (red line).
Figure S12. $\ln(C/C_0)$ versus time during the course of reduction of $p$-nitrophenol catalyzed by using excavated TOH Au NCs, cubic Au NCs and TOH Au NCs, respectively.