Supporting Information

Facile Synthesis of Concave Cuboid Au NCs with Precisely Tunable Dimensions and Mechanistic Insight

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Figure S1. FE-SEM image of CCB Au NCs synthesized using 2.5 μL of seed; scale bar is 200 nm.

Figure S2. (a) UV-vis spectra recorded for the CCB Au NCs synthesized with varying the amount of AgNO_3 as 10, 20, 30, 50, 70 and 100 μL while keeping the amount of seed (200 μL) constant. (b-g) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for all.

Figure S3. (a) UV-vis spectra recorded for the CCB Au NCs synthesized with varying the amount of AgNO_3 as 10, 20, 30, 50, 70 and 100 μL while keeping the amount of seed (100 μL) constant. (b-g) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for all.

Figure S4. (a) UV-vis spectra recorded for the CCB Au NCs synthesized with varying the amount of AgNO_3 as 10, 20, 30, 50 and 70 μL while keeping the amount of seed (50 μL) constant. (b-f) FE-SEM images were captured for the corresponding samples; scale bar is 100 nm for all.

Figure S5. (a) UV-vis spectra of CCB Au NCs synthesized with varying the amount of seed in the growth solution as 200, 100, 50, 10 μL in a 19:1 CTAC:CTAB growth solution. (b-e) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for all.

Figure S6. (a) UV-vis spectra of CCB Au NCs synthesized with varying the amount of seed in the growth solution as 200, 100, 50, 10 μL in a 1:1 CTAC:CTAB growth solution. (b-e) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for all.

Figure S7. (a) UV-vis spectra of CCBs synthesized in presence of BDAC and 1:1 CTAC:BDAC binary mixture. (b-c) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for both. d) UV-vis spectra of CCBs synthesized in presence of CPC and 1:1 CTAC:CPC binary mixture. (e-f) FE-SEM images were captured for the corresponding samples; scale bar is 200 nm for both.

Figure S8. (a) UV-vis spectra recorded at different time points from the addition of Au NRs seed, 120 min, 240 min, 360 min and 24 h (final) during the evolution of CCB Au NCs. (b-e) FE-SEM images were captured for the corresponding samples; scale bar is 100 nm for all.

Figure S9. HR-TEM images of the two intermediates (corresponding to Figure 5i and Figure 5j of Main Text) showing the concave morphology at the ends as well; scale bar is 2 nm for both.

Figure S10. (a) UV-vis spectra of Au NCs synthesized in presence of ascorbic acid (AA). (b) Corresponding FE-SEM image showing cuboids with concave faces; scale bar is 200 nm.

Figure S11. (a) UV-vis spectrum of one year old sample (prepared in May 2017) is very similar to the one recorded again in October 2018 (more than 1-year old). (b-c) Corresponding FE-SEM images taken in May 2017 (b) and in April 2019 (c), scale bar is 200 nm.

Figure S12. (a) CV traces recorded for CCB Au NCs with different sizes (see Figure 1b, d, f and h; 200 μL , 100 μL , 50 μL and 10 μL) in the presence of 0.5 M H_2SO_4 . (b) CV traces for the oxidation of 1 M HCOOH by CCB Au NCs with different sizes. (c) Plot of maximum current density vs length of CCB Au NCs showing a linear relationship.