Electronic Supplementary Information

Dodecahedral Au@Pd Nanocrystals with High-Index Facets and Excellent Electrocatalytic Activity and Highly Efficient Surface-Enhanced Raman Scattering Enhancement

Lei-fei Zhang and Chun-yang Zhang*

Single-Molecule Detection and Imaging Laboratory, Shenzhen Institutes of Advanced Technology,

Chinese Academy of Sciences, Shenzhen 518055, China



Figure S1. SEM and TEM images of 45-nm Au nanotriangles. The inset illustrates the

corresponding model of Au nanocrystal.

 Table S1. Theoretical projection angles and geometrical parameters of shield-like dodecahedral

| Geometrical model of polyhedron | Equation for the projection angle | Calculated projection angles | | | |
|------------------------------------|--|------------------------------|---------|---------|----------|
| α γ | $\alpha = 2\arctan(\frac{\sqrt{2}h}{k-l})$ | {hkl} | α | β | γ |
| | | {321} | 153.48° | 87.47° | 148.41 ° |
| | $\beta = 90 - (\frac{\alpha}{2}) + (\frac{\gamma}{2})$ | {431} | 141.06° | 98.05° | 157.16 ° |
| | $\gamma = 2 \arctan(\frac{h+k}{\sqrt{2}l})$ | {541} | 134.02° | 104.06° | 162.14 ° |
| | | {542} | 148.41° | 88.35° | 145.11 ° |
| | | {651} | 129.52° | 107.92° | 165.35 ° |

nanocrystals bounded by different high-index facets.



Figure S2. (a) Low- and (b) high-magnification TEM images of the shield-like Au@Pd nanocrystals. (c) HRTEM image taken from the region indicated with the red box in panel (b).



Figure S3. (a) TEM image of a shield-like Au@Pd nanocrystals viewed along the <110> direction.

(b) HRTEM image of the square region marked in (a) showing the {111} twin plane. (c) SEAD

patterns of the twin plane.



Figure S4. Energy-dispersive X-ray spectroscopy (EDS) spectrum of shield-shaped Au-Pd core-shell nanocrystals at different reaction time: 15 min (a) and 60 min (b).



Figure S5. UV-vis spectra of the reaction solution obtained at different reaction time.



Figure S6. TEM images of core-shell nanocrystals prepared with the molar ratio of $HAuCl_4/Na_2PdCl_4$ of 1:0 (a), 4:1 (b), 3:2 (c), 2:3 (d), 1:4 (e), and 0:1 (f).



Figure S7. SEM images of nanocrystals prepared with different volumes of ascorbic acid (0.1 M):

0.15 mL (a), 0.25 mL (b), 0.35 mL (c), and 0.50 mL (d).



Figure S8. SEM images of Au seeds obtained by the addition of (a) DDAB, (b) CTAC, (c) DDAB

+ CTAC, respectively.



Figure S9. (a-c) SEM and TEM images of cubic Au@Pd core-shell nanocrystals. (d-f) SEM and

TEM images of octahedral Au@Pd core-shell nanocrystals.