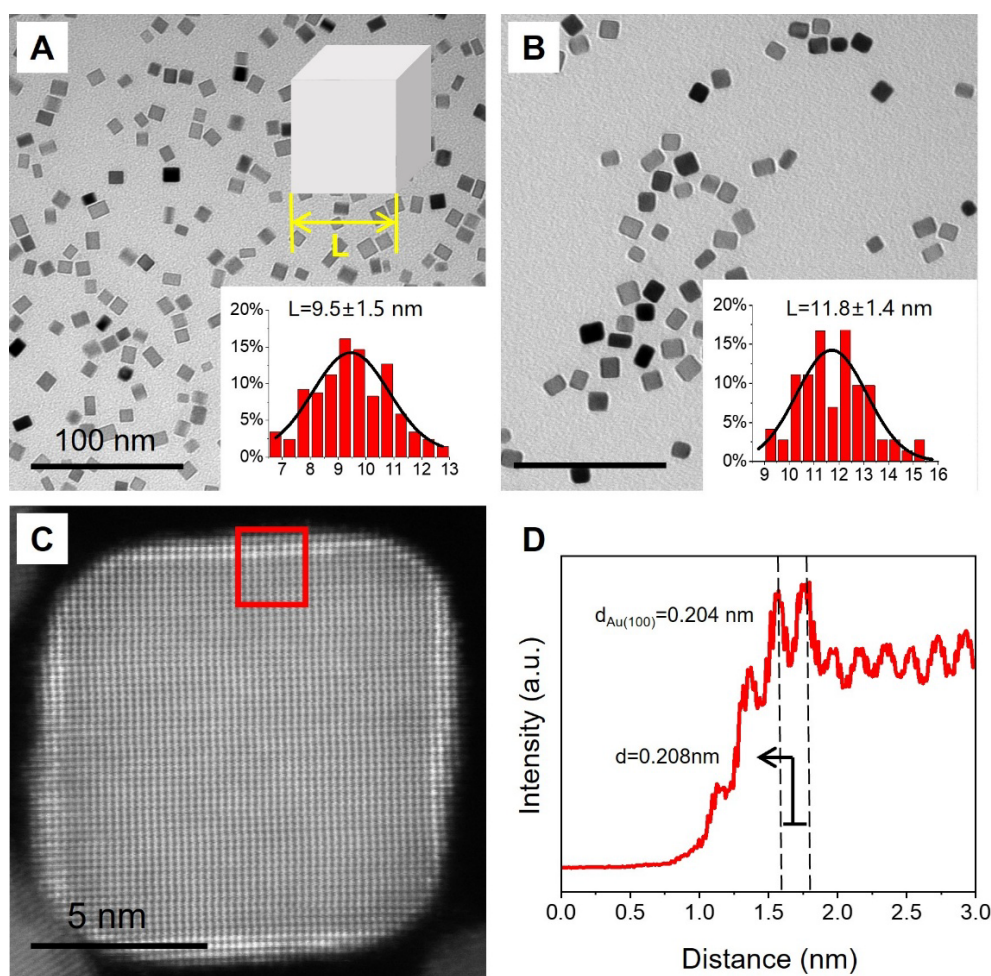


## Supplementary Materials

# Trimetallic Pd@Pt<sub>x</sub>Au<sub>1-x</sub> Core-Shell Nanocubes with Enhanced Selectivity toward H<sub>2</sub>O<sub>2</sub> for the Oxygen Reduction Reaction

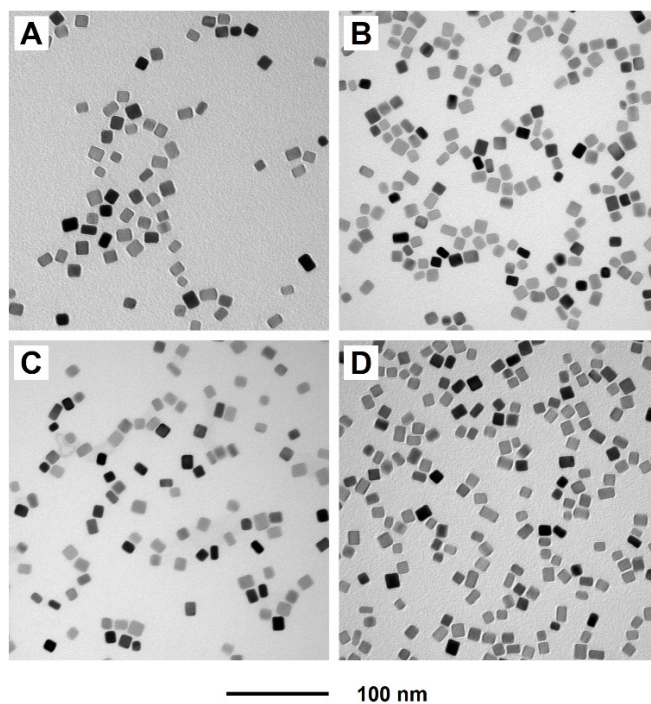
Zhiqi Wang<sup>1</sup>, Kei Kwan Li<sup>1</sup>, Yong Ding<sup>2</sup>, and Younan Xia<sup>1,3,\*</sup><sup>1</sup> School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332, USA<sup>2</sup> School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA<sup>3</sup> The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, GA 30332, USA

\* Correspondence: younan.xia@bme.gatech.edu

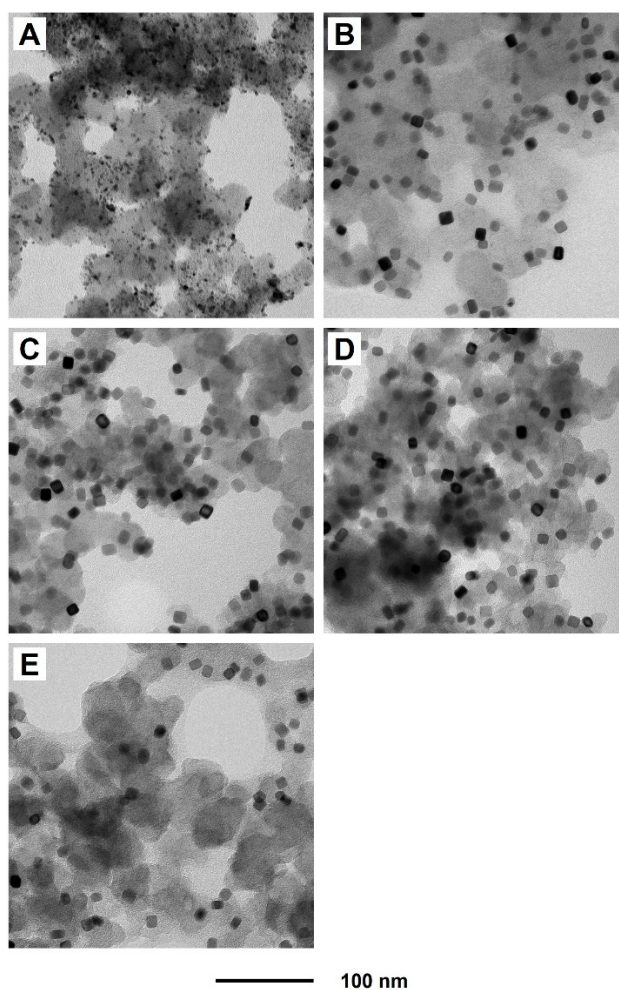


**Figure S1.** Synthesis of Pd and Pd@Au core-shell nanocubes. (A) TEM image of Pd nanocubes (together with size distribution in the inset); (B) TEM image of Pd@Au nanocubes (together with size distribution in the inset); (C) STEM image of a Pd@Au core-shell nanocube; and (D) Line scans of the Pd@Au core-shell nanocubes in the region of red line in (C). The scale bar in (A) applies to panel (B).





**Figure S2.** Variation of the feeding molar ratio between the Pt and Au precursors. TEM image of Pd@Pt<sub>x</sub>Au<sub>1-x</sub> core-shell nanocubes obtained with the Pt:Au precursor molar ratio being set to (A) 0:1; (B) 0.025:0.975; (C) 0.05:0.95; and (D) 0.1:0.9. The scale bar at the bottom applies to all panels.



**Figure S3.** TEM images of (A) commercial Pt/C catalyst and carbon-supported Pd@Pt<sub>x</sub>Au<sub>1-x</sub> nanocubes obtained with the Pt:Au precursor molar ratio being set to (B) 0:1; (C) 0.025:0.975; (D) 0.05:0.95 and (E) 0.1:0.9. The scale bar at the bottom applies to all panels.

**Table S1.** The Pt:Au atomic ratio in Pd@Pt<sub>x</sub>Au<sub>1-x</sub> nanocubes as derived from ICP-MS data.

Sample	Pt:Au Atomic Ratio by ICP Data	Pt Mass Percent in the Particle (%)
Pd@Au	0:1.000	0
Pd@Pt <sub>0.025</sub> Au <sub>0.975</sub>	0.001:0.999	0.02
Pd@Pt <sub>0.025</sub> Au <sub>0.975</sub>	0.018:0.982	0.35
Pd@Pt <sub>0.1</sub> Au <sub>0.9</sub>	0.027:0.973	0.42

**Table S2.** Summary of the XPS peak positions (unit: eV) of Pd and core-shell nanocubes.

Sample	Pd3d5/2	Pd3d3/2	Au4f7/2	Au4f5/2	Pt4f7/2	Pt4f5/2
Pd	333.9	339.2	—	—	—	—
Pd@Au	333.9	339.2	82.4	86.1	—	—
Pd@Pt <sub>0.025</sub> Au <sub>0.975</sub>	333.7	338.9	82.2	85.9	69.6	72.8
Pd@Pt <sub>0.05</sub> Au <sub>0.95</sub>	333.5	338.8	82.0	85.7	69.4	72.9
Pd@Pt <sub>0.1</sub> Au <sub>0.9</sub>	333.4	338.7	82.0	85.6	69.7	72.8