Supporting Information

## Investigating Lattice Strain Impact on the Alloyed Surface of Small Au@PdPt Core-Shell Nanoparticles

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**Figure S1.** TEM images of  $Pd_1Pt_1$  nanoparticles made by bubbling with oxygen gas.

Most particles are octahedral but larger in size than those made with argon bubbling, suggesting that the slow reaction rate allows {111} crystal facets to dominate during particle growth.



Figure S2. Photographs of alloy and core-alloyed shell octahedral nanoparticles.



**Figure S3.** Size dispersions of alloy and core-alloyed shell nanoparticles. Histograms of (a, c, e) PdPt alloy and (b, d, f) Au-PdPt core-alloyed shell nanoparticles, with (f-h) representing the Au-Pd<sub>1</sub>Pt<sub>3</sub> core-shell nanoparticles with different thicknesses.





TEM images and histogram showing the octahedral Au seeds are 8.2 nm and truncated on their corners.



**Figure S5.** Formic acid oxidation cyclic voltammograms for Pd:Pt study. Polarization curves of formic acid oxidation on PdPt alloy and Au-PdPt core-shell octahedral nanoparticles.



**Figure S6.** Formic acid oxidation cyclic voltammograms for thickness study. Polarization curves of formic acid oxidation on  $Au-Pd_1Pt_3$  core-shell nanoparticles with thickness (a) 1.3 nm, (b) 2.3 nm), (c) 3.5 nm, and  $Pd_1Pt_3$  alloy nanoparticles with the size (d) 7.8 nm.



**Figure S7.** Synchrotron-based XRD analysis of Au seeds. Synchrotron-based XRD pattern of Au seeds with (220) peak standing at 42.09°.

molar ratio (Pd <sup>2+</sup> : Pt <sup>2+</sup> )	Pd (atomic %)	Pt (atomic %)	Composition		
3:1	19.39	7.56	$Pd_{2.6}Pt_{1.0}$		
1:1	13.45	13.12	Pd <sub>1.0</sub> Pt <sub>1.0</sub>		
1:3	5.60	13.10	Pd <sub>1.0</sub> Pt <sub>2.4</sub>		

 Table S1. EDS-analyzed composition of octahedral alloy nanoparticles.

molar ratio (Pd <sup>2+</sup> : Pt <sup>2+</sup> )	Pd (atomic %)	Pt (atomic %)	Composition
3:1	20.08	7.39	Au@Pd <sub>2.7</sub> Pt <sub>1.0</sub>
1:1	18.18	14.22	Au@Pd <sub>1.3</sub> Pt <sub>1.0</sub>
1:3	6.03	15.12	Au@Pd <sub>1.0</sub> Pt <sub>2.5</sub>

 Table S2. EDS-analyzed composition of octahedral Au-PdPt core-shell nanoparticles.

Thickness (nm)	Pd (atomic %)	Pt (atomic %)	Composition		
1.3	1.80	5.21	Au@Pd <sub>1.0</sub> Pt <sub>2.9</sub>		
2.3	6.03	15.12	Au@Pd <sub>1.0</sub> Pt <sub>2.5</sub>		
3.5	3.34	8.23	Au@Pd <sub>1.0</sub> Pt <sub>2.5</sub>		

**Table S3.** Composition of  $Au-Pd_1Pt_3$  core-shell octahedral nanoparticles with different thickness.

Pdª	<b>Pt</b> <sup>b</sup>	Pd <sub>1</sub> Pt <sub>2.4</sub> (7.8 nm)		Au-Pd₁Pt <sub>2.5</sub> (3.5 nm)		Au-Pd <sub>1</sub> Pt <sub>2.5</sub> (2.3 nm)		Au-Pd₁Pt <sub>2.9</sub> (1.3 nm)	
<b>a</b> ° <sub>Pd</sub>	<b>a</b> ° <sub>Pt</sub>	<b>a</b> ° <sub>PdPt</sub> c	<b>a</b> <sub>PdPt</sub> <sup>d</sup>	<b>a</b> ° <sub>PdPt</sub>	<b>a</b> <sub>PdPt</sub>	<b>a</b> ° <sub>PdPt</sub>	<b>a</b> <sub>PdPt</sub>	<b>a</b> ° <sub>PdPt</sub>	<b>a</b> <sub>PdPt</sub>
3.867*	3.920	3.904	3.903	3.905	3.915	3.905	3.925	3.906	3.940
		δ <sub>S</sub> <sup>e</sup> = –(	0.02 %	δ <sub>S</sub> = 0.2	26 %	δ <sub>S</sub> = 0.8	51 %	δ <sub>S</sub> = 0.8	37 %

Table S4. Lattice parameters and strain of Pd, Pt, Pd1Pt3 alloy, and Au-Pd1Pt3 coreshell nanoparticles with different shell thickness.

\* All lattice parameters are given in Å.

*a*, *b* Lattice parameters  $a_{PdPt}^{\circ}$  and  $a_{Pt}^{\circ}$  are referred to x-ray diffraction database no. 87-0645 and no. 87-0646. *c*  $a_{PdPt}^{\circ}$  of the alloy Pd<sub>x</sub>Pt<sub>1-x</sub> is the estimated lattice parameter got by Vegard's law in which  $a_{PdPt}^{\circ}$  is the sum of  $xa_{Pd}^{\circ}$  and  $(1-x)a_{Pt}^{\circ}$ .

*d a*<sub>PdPt</sub> is the experimental lattice parameter obtained from (220) peaks in synchrotron-based XRD patterns.

e δ<sub>S</sub> is lattice strain calculated by  $[(a_{PdPt} - a_{PdPt}^{\circ})/a_{PdPt}^{\circ}] \times 100$  (%).