Supplementary

Ultra-small nanoparticles of Pd-Pt-Ni alloy octahedra with high lattice strain for efficient oxygen reduction reaction

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Supplementary Figures S1-S4

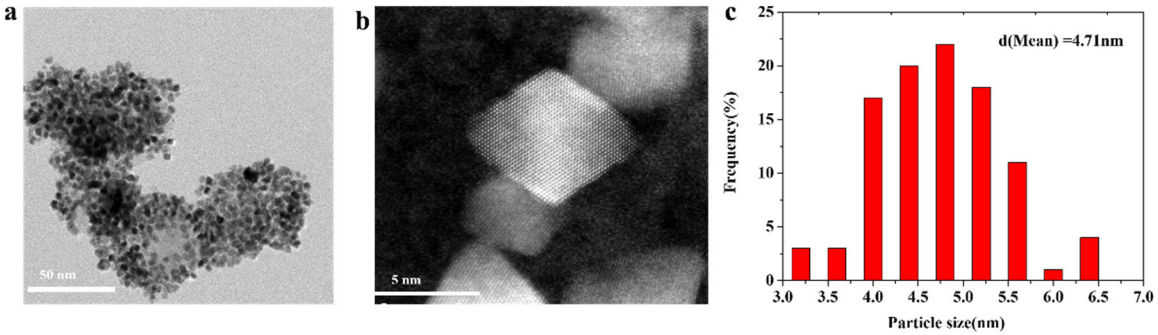

Figure. S1. (a-b) TEM image of Pd-Pt-Ni Octa1. (c) corresponding particle size distribution.

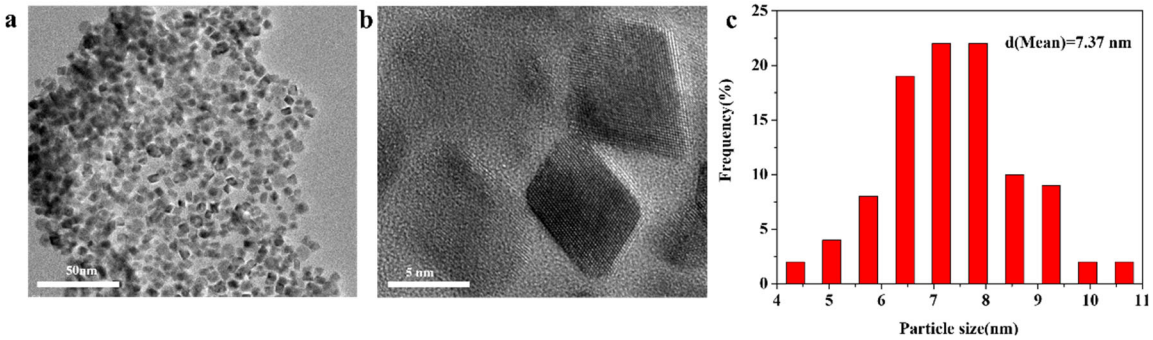

Figure. S2. (a-b) TEM image of Pd-Pt-Ni Octa2 (c) corresponding particle size distribution.

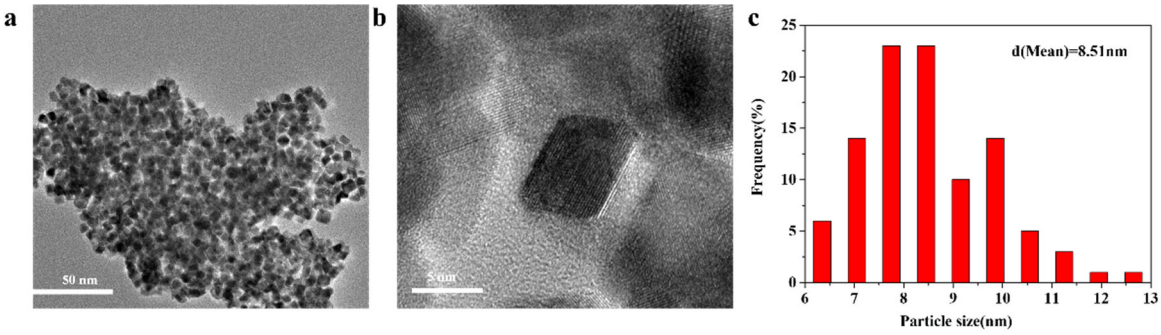

Figure. S3. (a-b) TEM image of Pd-Pt-Ni Octa3 (c) corresponding particle size distribution.

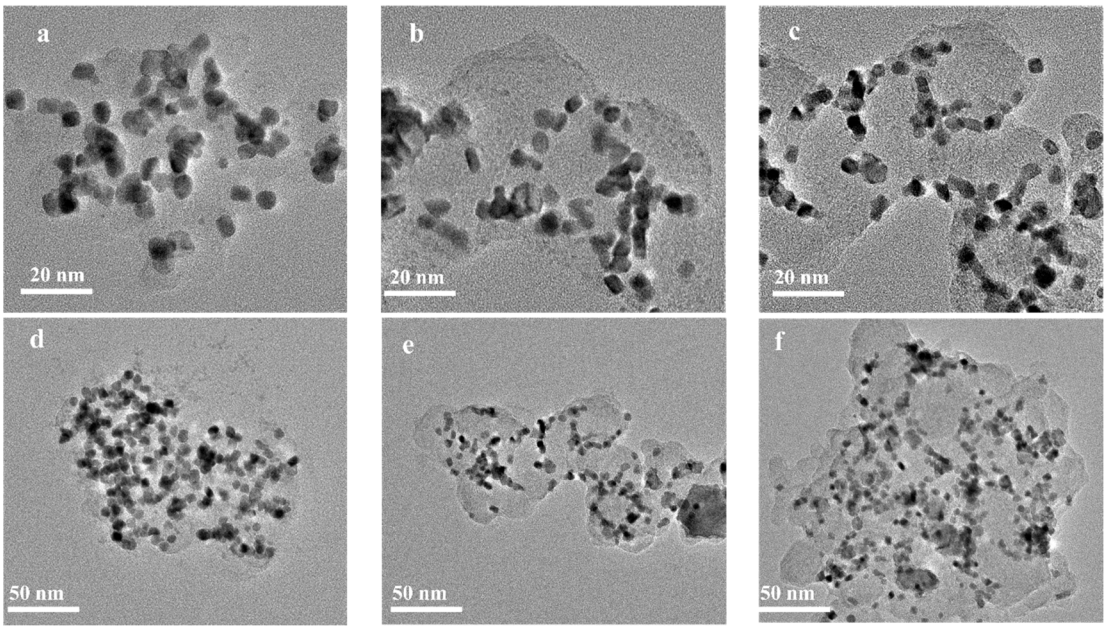

Figure.S4. (a-f) TEM images after 10k cycles of Pd-Pt-Ni Octa1

Supplementary Tables S1-S6

Table S1. Pt, Pd and Ni atomic ratio examined of Pd-Pt-Ni Octa1，Pd-Pt-Ni Octa2，Pd-Pt-Ni Octa3 by XPS and ICP-OES.

Samples	XPS (Pt%/ Pd%/ Ni%)	ICP-OES (Pt%/ Pd%/ Ni%)
Pd-Pt-Ni Octa1	67.8/19.5/12.6	58.4/35.8/5.7
Pd-Pt-Ni Octa2	63.7/16.5/19.7	55.3/37.4/7.2
Pd-Pt-Ni Octa3	38.1/14.9/47.1	55.3/37.3/7.4

Table S2. The relevant Lattice parameter correlated to Pt(111) plane (nm) and calculated strain of Pt，Pd-Pt-Ni Octa1，Pd-Pt-Ni Octa2 and Pd-Pt-Ni Octa3.

Sample	XRD	Strain (%)	FFT	Strain (%)	VASP	Strain (%)
Pt	0.2265	------	0.2265	------	0.2807	------
Pd-Pt-Ni Octa1	0.2239	1.14	0.2160	4.63	0.2709	3.49
Pd-Pt-Ni Octa2	0.2250	0.67	0.2220	1.98	------	------
Pd-Pt-Ni Octa3	0.2258	0.31	0.2236	1.28	------	------

Table S3. When the gas phase water was at 0.035 bar and T=298 K, the gas phase water was in equilibrium with liquid water. The following data are calculated at this equilibrium state.

Species	E (eV)	ΔG(T) (eV)	G (eV)
O_2(g)			-9.72
H_2(g)	-6.77	-0.04	-6.81
H_2O(l)	-14.22	0.09	-14.13

Table S4. Gibbs free energy in a four-electron reaction，while product1 stands for 2 (H^++e^-) +H_2O and product2 stands for H^++e^-+H_2O，U=0 V

Matrix	ΔG($2H_2$+O_2) (eV)	ΔG(*OOH+product1) (eV)	ΔG(*O+product2) (eV)	ΔG(*OH+product3) (eV)	ΔG($2H_2O$) (eV)
Pt (111)	4.80	4.09	1.81	1.12	0
Pd-Pt-Ni Octa1(111)	4.80	4.02	1.71	1.05	0

Table S5: In the four-electron reaction, the **Gipps free energy of Pd-Pt-Ni Octa1 (111) in ORR** each step at 1.23V is as follows: ΔG(H_2O) = 0, ΔG(*OH) = 1.12-1.23, ΔG(*O) = 1.81 - 2*1.23, ΔG(*OOH) = 4.09 - 3*1.23, ΔG(O_2) = 4.8 - 4*1.23.

In the four-electron reaction, the **Gipps free energy of Pt/C in ORR** each step at 1.23V is as follows: ΔG(H_2O) = 0, ΔG(*OH) = 1.05 - 1.23, ΔG(*O) = 1.71 - 2*1.23, ΔG(*OOH) = 4.02 - 3*1.23, ΔG(O_2) = 4.8 - 4*1.23.

Matrix	ΔG($2H_2$+O_2) (eV)	ΔG(*OOH+product1) (eV)	ΔG(*O+product2) (eV)	ΔG(*OH+product3) (eV)	ΔG($2H_2O$) (eV)
Pt (111)	-0.12	0.40	-0.65	-0.11	0
Pd-Pt-Ni Octa1(111)	-0.12	0.33	-0.75	-0.18	0

Table S6. Performance of Pd-Pt-Ni Octa1, Pd-Pt-Ni Octa2 and Pd-Pt-Ni Octa3 catalyst compared to Pt/C.

Catalyst	Half-wave potential $E_{1/2}$ (V)	Mass activity (A mg_{Pt}^{-1}) at 0.9 V vs RHE	Mass activity (A mg_{Pt+Pd}^{-1}) at 0.9 V vs RHE	Mass activity after ADT (A mg_{Pt}^{-1}) at 0.9V *vs* RHE
Pd-Pt-Ni Octa1	0.933	1.55	0.93	0.51
Pd-Pt-Ni Octa2	0.917	0.75	0.48	------
Pd-Pt-Ni Octa3	0.910	0.70	0.40	-------
Pt/C	0.897	0.16	------	0.09