Supporting information

# Optimizing the Oxygen Reduction Reaction Activity of Pd Based Nanocatalyst by Tuning Strain and Particle Size

Weiping Xiao,[a] Marco Aurelio Liutheviciene Cordeiro,[b] Mingxing Gong, [a] Lili Han, [c] Jie Wang,[a] Ce Bian,[a] Jing Zhu,[a] Huolin Xin,[b] and Deli Wang [a,]*

**Table S1** The ICP-AES results of $Pd_2FeCo$@Pt/C catalyst.

| $Pd_2FeCo$@Pt/C | Weight ratio | Atom ratio |
|---|---|---|
| Pt:Pd:Fe:Co-initial | 2.7:100:23.0:25.5 | 1.5:100: 43.7:46.0 |
| Pt:Pd:Fe:Co-ADT | 3.1:100:21.7:23.5 | 1.7:100: 41.2:42.3 |

**Table S2** Comparison of MA at 0.9 V for Pd(Au)M@Pt and Pt/C extracted from literature.

| Catalysts | MA at 0.9 $V_{RHE}$ | MA (Pt/C) at 0.9 $V_{RHE}$ | Electrolyte | Refs |
|---|---|---|---|---|
| $Pd@Pt_{2\text{-}3L}$ | 0.49 A $mg_{Pt}^{-1}$ | 0.1 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 1 |
| Pd(core)-Pt(shell) | 0.2 A $mg_{Pt}^{-1}$ | 0.12 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 2 |
| $Pd@Pt_{1L}$ | 0.35 A $mg_{Pt}^{-1}$ | 0.12 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 3 |
| Pd@Pt | 1.6 A $mg_{Pt}^{-1}$ | 0.32 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 4 |
| $Pd@Pt_{1.8}Ni$ | 0.8 A $mg_{Pt}^{-1}$ | 0.16 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 5 |
| $Pt_{ML}/Pd_9Au_1$ | 0.31 A $mg_{Pt}^{-1}$ | 0.1 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 6 |
| Pd@Pt | 1.56 A $mg_{Pt}^{-1}$ | 0.081 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 7 |
| $Pd_3Au@Pt$ | 0.94 A $mg_{Pt}^{-1}$ | 0.203 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 8 |
| AuCu@Pt | 0.56 A $mg_{Pt}^{-1}$ | 0.098 A $mg_{Pt}^{-1}$ | 0.5 M $H_2SO_4$ | 9 |
| AuCu@Pt | 0.57 A $mg_{Pt}^{-1}$ | 0.11 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 10 |
| Pd@Pt-Ni | 2.5 A $mg_{Pt}^{-1}$ | 0.2 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 11 |
| $Pd_8CoZn@Pt$ | 2.18A $mg_{Pt}^{-1}$ | 0.07 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | 12 |
| Pd@Pt | 0.24 A $mg_{Pt}^{-1}$ | 0.1 A $mg_{Pt}^{-1}$ | 0.1 M KOH | 13 |
| AuCu@Pt | 0.86A $mg_{Pt}^{-1}$ | 0.088 A $mg_{Pt}^{-1}$ | 0.1 M KOH | 14 |
| $Pd_2FeCo@Pt$ | 2.5 A $mg_{Pt}^{-1}$ | 0.066 A $mg_{Pt}^{-1}$ | 0.1 M $HClO_4$ | This work |
| $Pd_2FeCo@Pt$ | 5.4 A $mg_{Pt}^{-1}$ | 0.048 A $mg_{Pt}^{-1}$ | 0.1 M KOH | This work |

**Table S3** Comparison of key performance parameters for Zn-air batteries extracted from literature.

| Catalysts | Loading (mg $cm^{-2}$) | Peak power density | Electrolyte | Refs |
|---|---|---|---|---|
| CuPt-NC | 2.0 | 250 mW $cm^{-2}$ | 6 M KOH | 15 |
| $Pb_2Ru_2O_{6.5}$ | — | 195 mW $cm^{-2}$ | 6 M KOH + 0.2 M ZnO | 16 |
| P,S-CNS | 0.5 | 198 mW $cm^{-2}$ | 6 M KOH | 17 |
| S-DGF | — | 300 mW $cm^{-2}$ | 6 M KOH + 0.2 M $ZnCl_2$ | 18 |
| C–CoPAN900 | 1.0 | 125 mW $cm^{-2}$ | 6 M KOH +0.2 M $ZnCl_2$ | 19 |
| CoO/N-CNT+NiFe LDH/CNT | 1.0 | 265 mW $cm^{-2}$ | 6 M KOH + 0.2 M zinc acetate | 20 |
| Co@NG-acid | 1.0 | 350 mW $cm^{-2}$ | 6 M KOH | 21 |
| CuFe alloy | | 212 mW $cm^{-2}$ | 6 M KOH | 22 |
| $NiCo_2S_4$/N-CNT | 1.0 | 147 mW $cm^{-2}$ | 6 M KOH + 0.2 M $ZnCl_2$ | 23 |
| CoFe@NCNTs | 1.0 | 150 mW $cm^{-2}$ | 6 M KOH + 0.2 M zinc acetate | 24 |
| $Pd_2FeCo$/C | 1.0 | 256 mW $cm^{-2}$ | 6 M KOH + 0.2 M zinc acetate | This work |
| $Pd_2FeCo$@Pt/C | 1.0 | 308 mW $cm^{-2}$ | 6 M KOH + 0.2 M zinc acetate | This work |

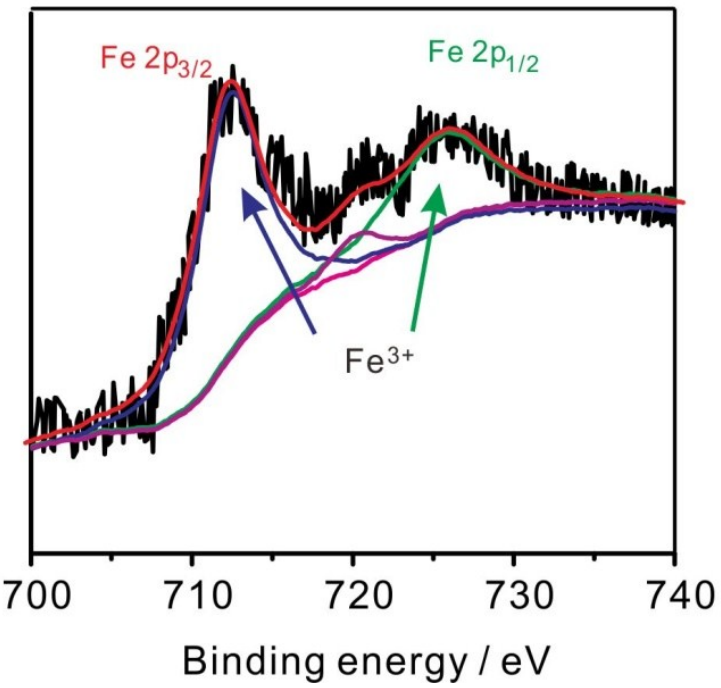


**Fig. S1** XPS curves of Fe on $Pd_2FeCo/C$ nanoparticles.

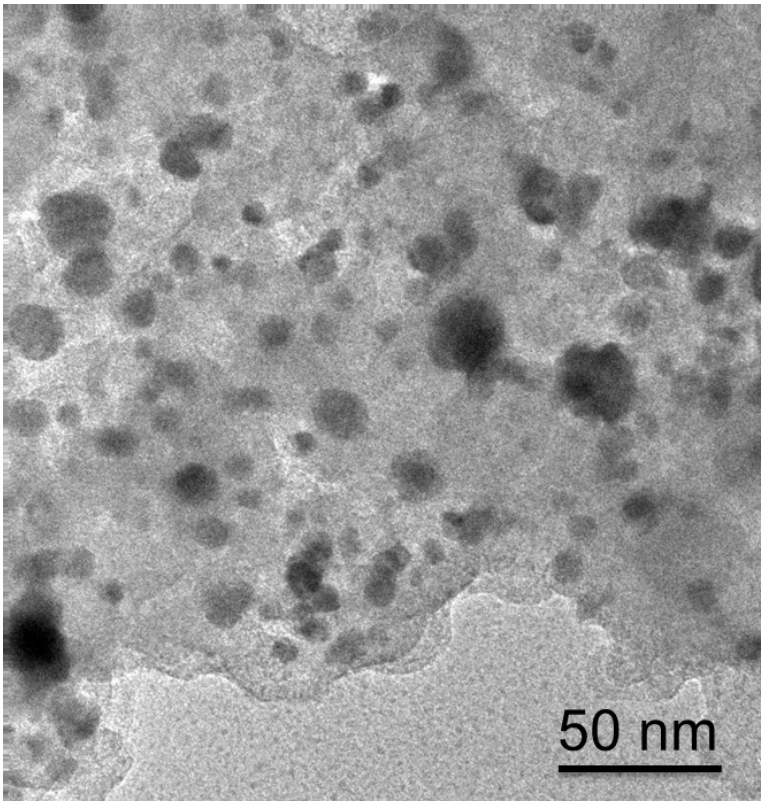


**Fig. S2** Overview STEM image of PdFe/C nanoparticles.

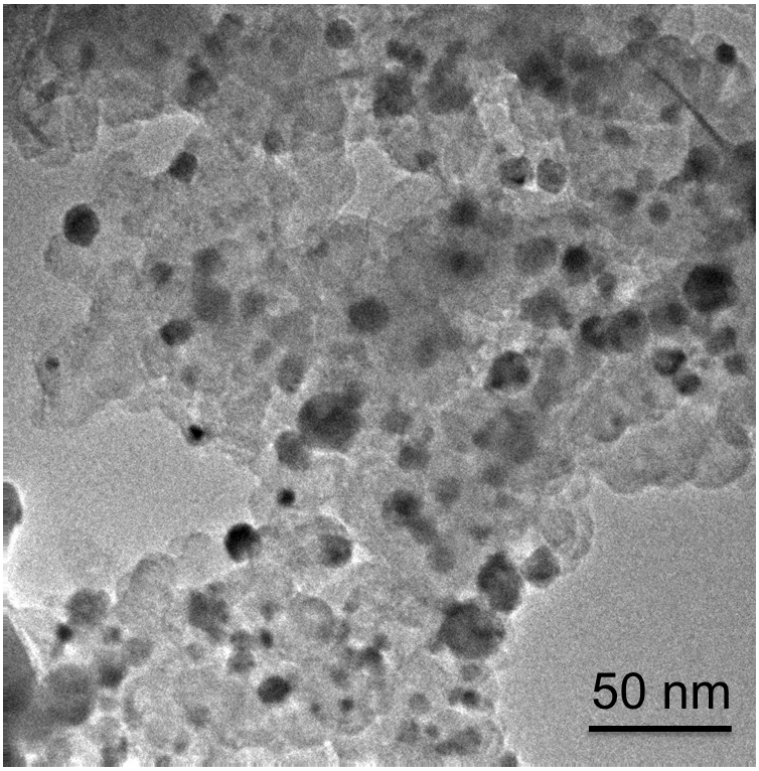


**Fig. S3** Overview STEM image of PdCo/C nanoparticles.

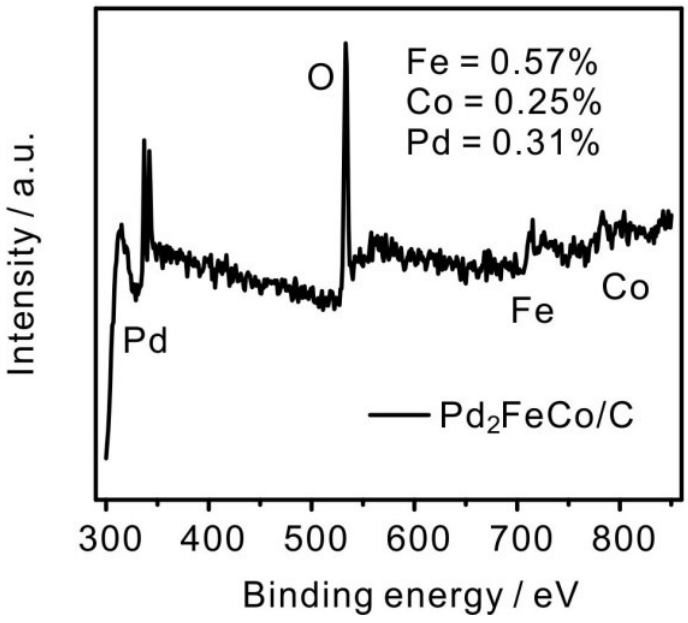


**Fig. S4** XPS curves of $Pd_2FeCo/C$ nanoparticles.

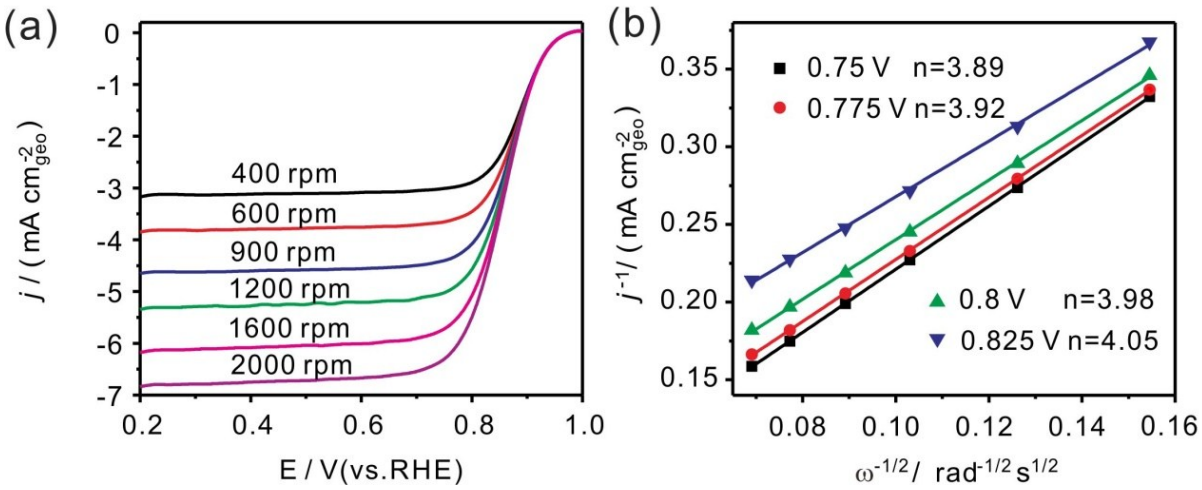


**Fig. S5** (a) The rotation-rate-dependent current-potential curves of $Pd_2FeCo/C$. (b) The Koutecky-Levich plots on $Pd_2FeCo/C$ at different potentials.

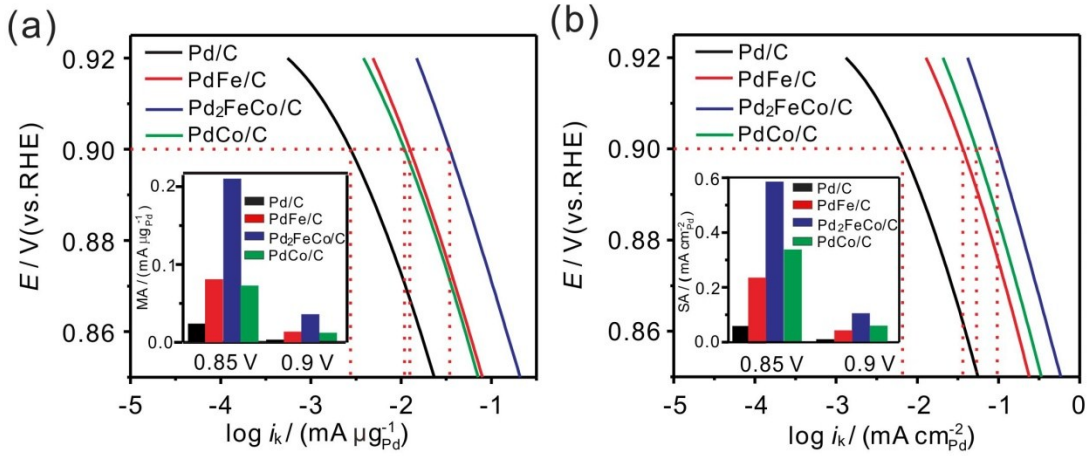


**Fig. S6** (a) Mass activities and (b) specific activities at 0.85 V and 0.9 V, respectively.

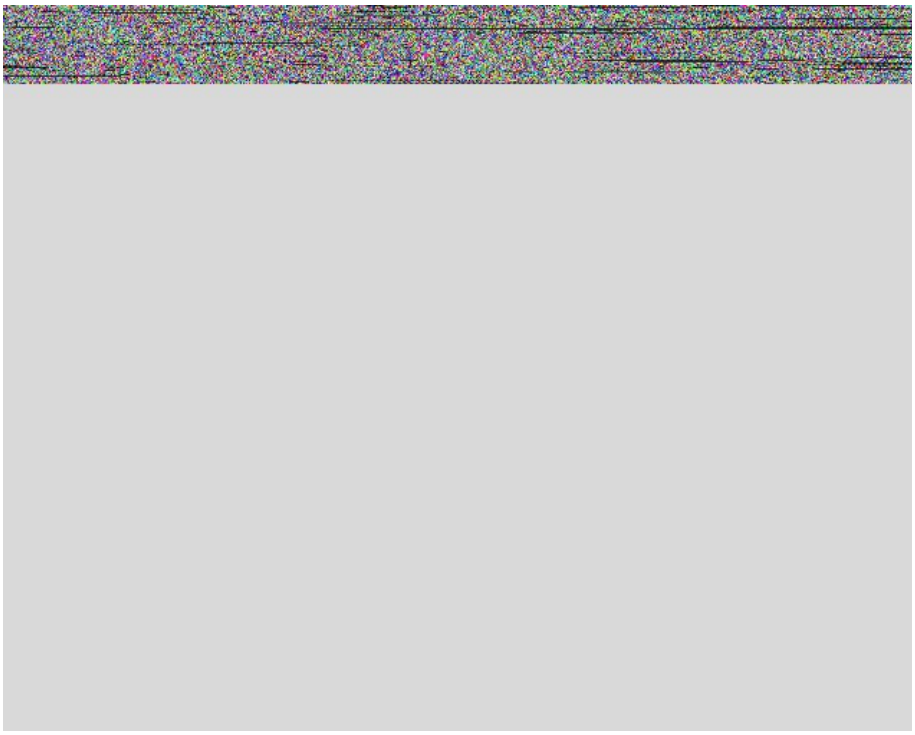

**Fig. S7** CV curves of Pd/C, PdFe/C, PdCo/C and $Pd_2FeCo$/C in $N_2$-saturated 0.1 M $HClO_4$ solution, sweep rate, 50 mV $s^{-1}$.

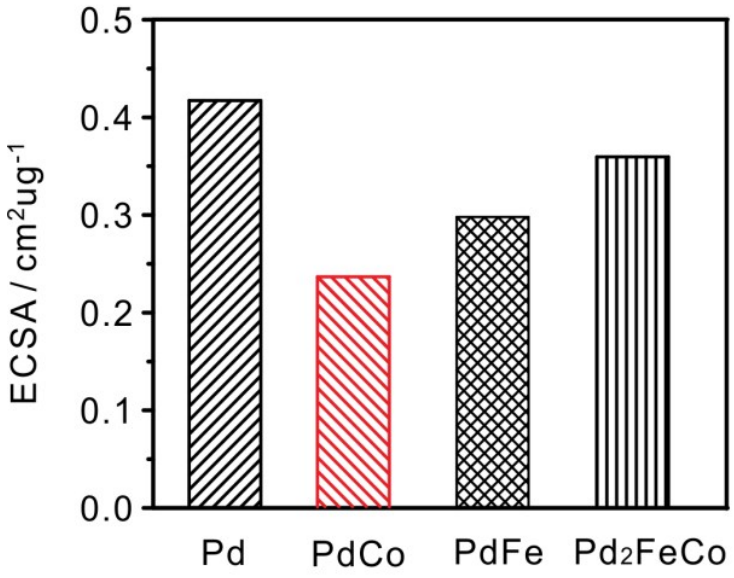


**Fig. S8** ECSA of Pd/C, PdFe/C, PdCo/C and $Pd_2FeCo$/C catalysts.

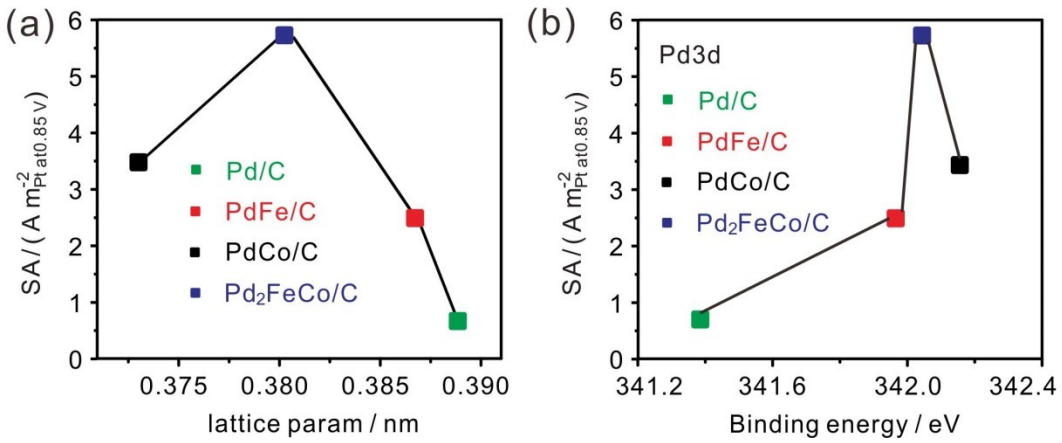


**Fig. S9** The relationship between specific activity and lattice constant (a), binding energy (b) of Pd.

**Fig. S10** ORR polarization curves of $Pd_2FeCo/C$-300 and $Pd_2FeCo/C$-500.

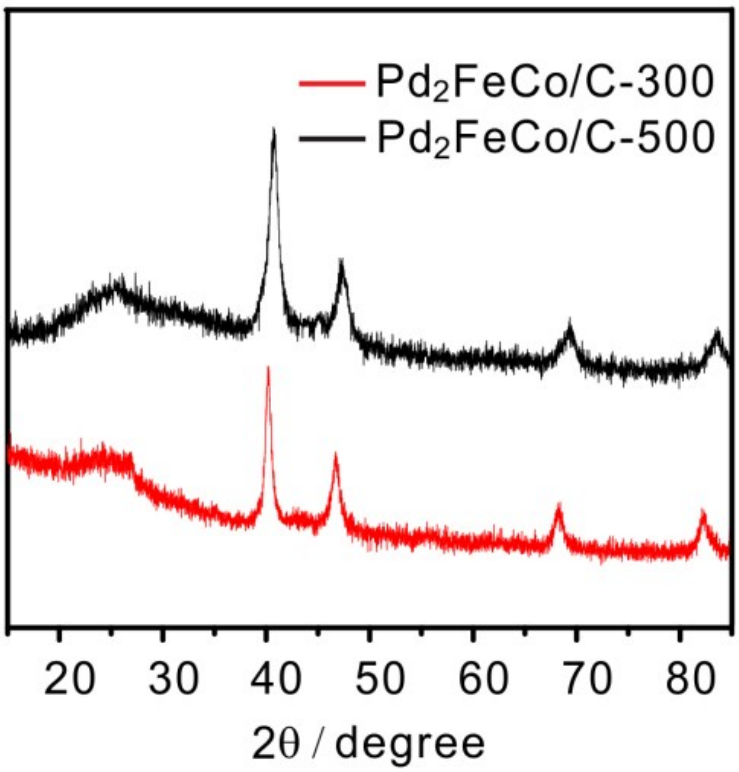


**Fig. S11** XRD patterns of $Pd_2FeCo$/C-300 and $Pd_2FeCo$/C-500.

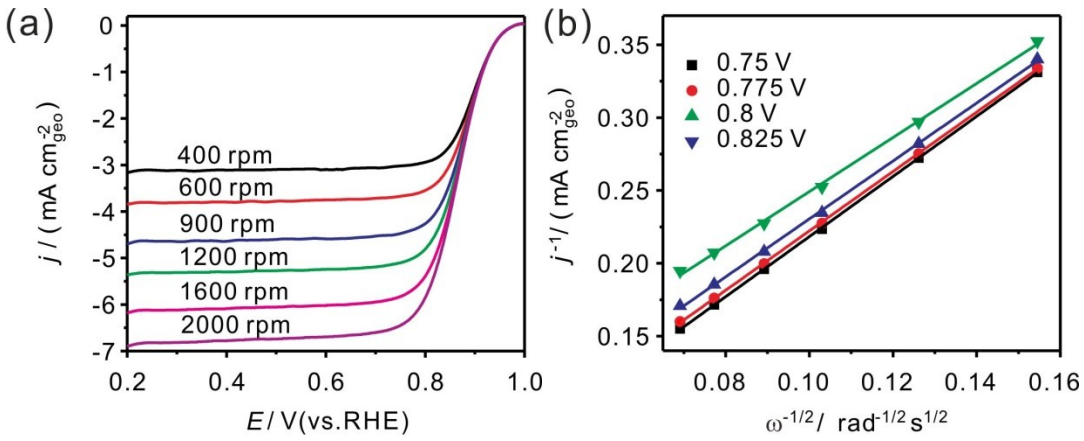


**Fig. S12** (a) The rotation-rate-dependent current-potential curves of $Pd_2FeCo$@Pt/C. (b) The Koutecky-Levich plots on $Pd_2FeCo$@Pt/C at different potentials.

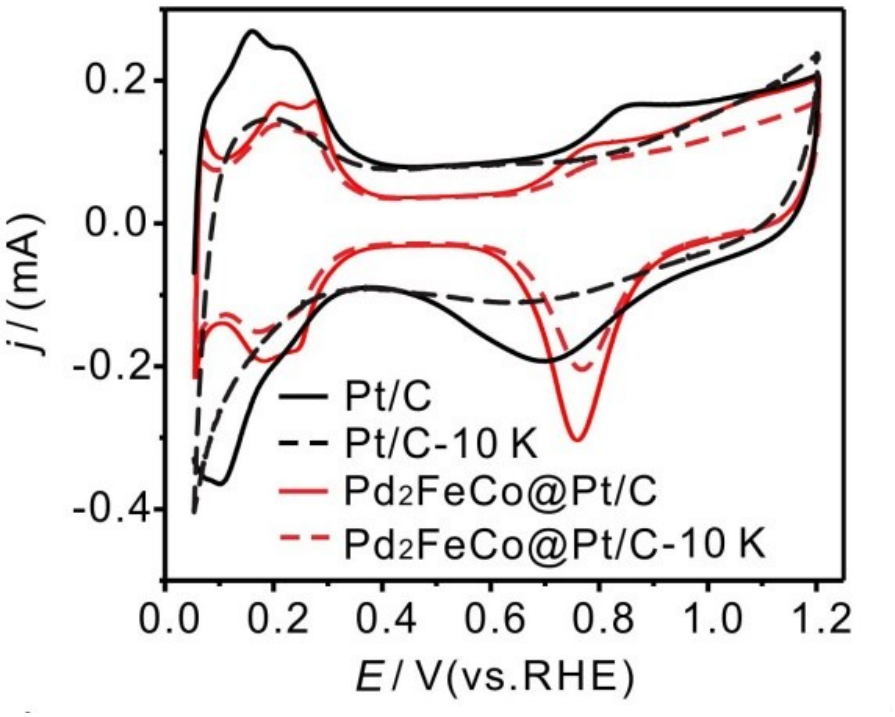


**Fig. S13** CV curves of $Pd_2FeCo$@Pt/C and Pt/C nanoparticles before and after 10, 000 cycles durability test in 0.1 M $N_2$-saturated $HClO_4$, sweep rate, 50 mV $s^{-1}$.

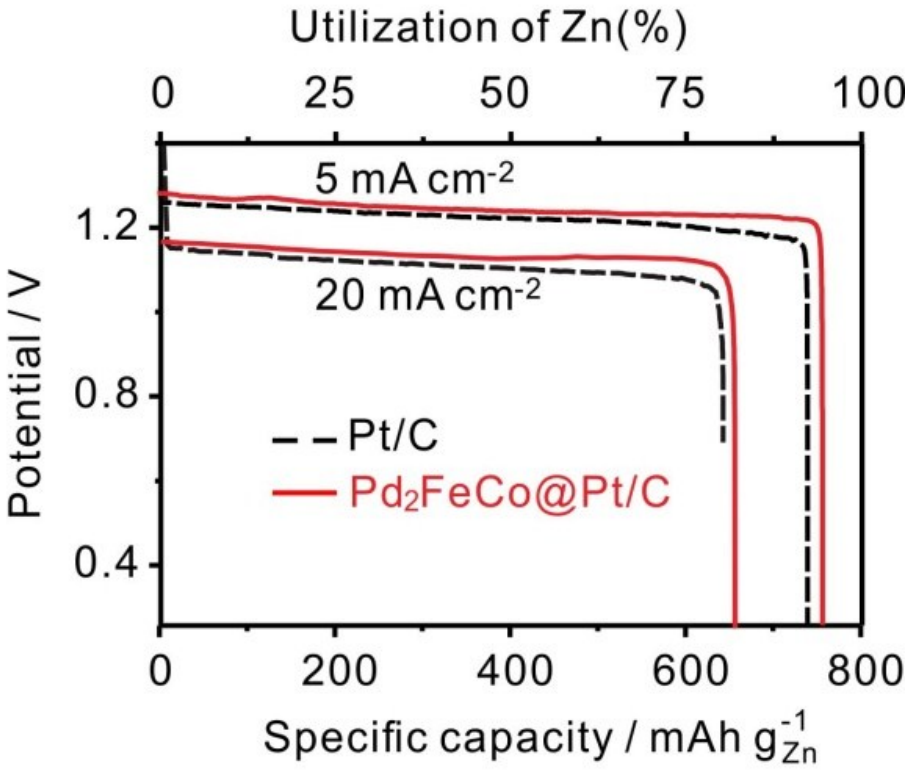


**Fig. S14** Specific capacities of the Zn-air batteries using $Pd_2FeCo$@Pt/C and Pt/C as ORR catalyst at current densities of 5 and 20 mA $cm^{-2}$.

References


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