

Supporting Information

Platinum-Palladium Alloy Nanotetrahedra with Tuneable Lattice-Strain for Enhanced Intrinsic Activity

Ruifang Miao^{a#}, Fangfang Chang^{a#, *}, Mengyun Ren^a, Xianhong He^a, Lin Yang^{a*}, Xiaolei Wang^b and Zhengyu Bai^{a*}

^a Collaborative Innovation Center of Henan Province for Green Manufacturing of Fine Chemicals, Key Laboratory of Green Chemical Media and Reactions, Ministry of Education, School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 453007, China. Email: changfangfang@htu.edu.cn; yanglin@htu.edu.cn; baizhengyu@htu.edu.cn

^b Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta T6G 1H9, Canada.

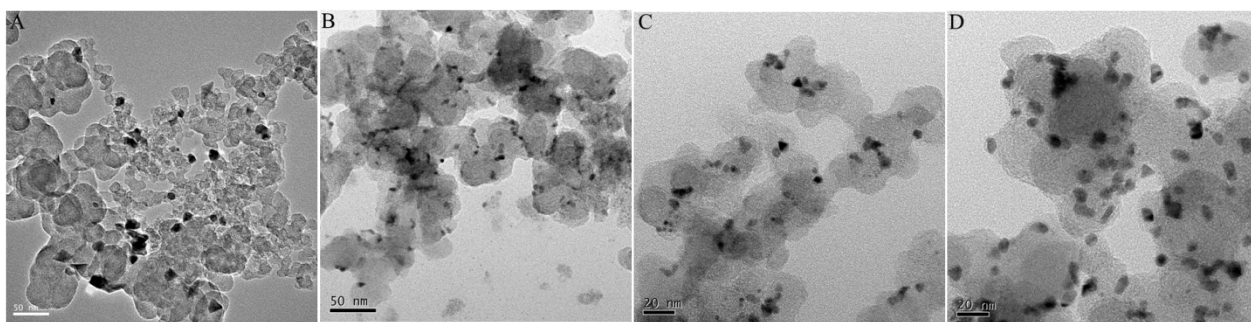


Fig. S1 TEM images of the nanotetrahedra samples ((A) Pt₁₆Pd₈₄/C, (B) Pt₃₅Pd₆₅/C, (C) Pt₈₃Pd₁₇/C and (D) Pt NPs/C).

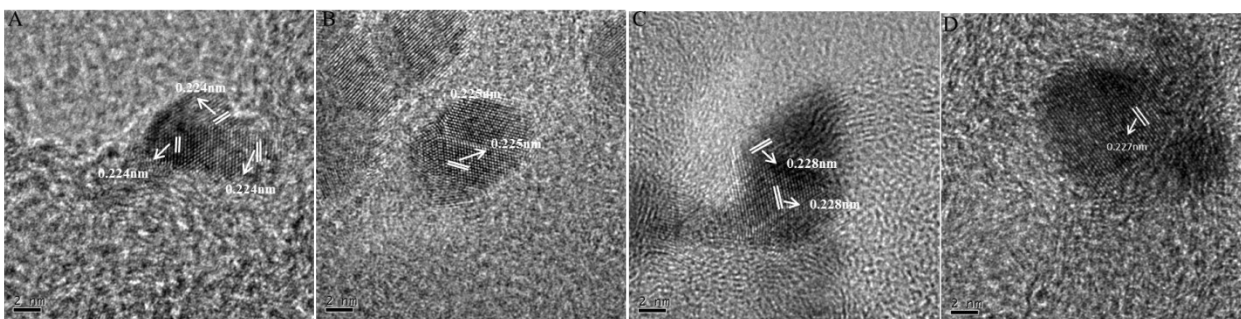


Fig. S2 HR-TEM images of the nanotetrahedra samples ((A) Pt₁₆Pd₈₄/C, (B) Pt₃₅Pd₆₅/C, (C) Pt₈₃Pd₁₇/C and (D) Pt NPs/C).

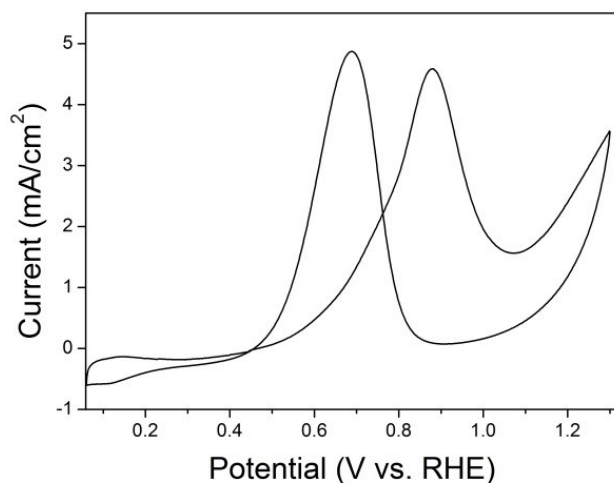


Fig. S3 CV curve of commercial Pt/C in 0.1 M HClO₄ + 0.5 M CH₃OH solution purged with N₂ at a scan rate of 50 mV s⁻¹

Table S1 Comparison of MOR activities of various catalysts

Catalyst	Electrolyte	Mass Activity (A/mg _{Pt} ⁻¹)	Specific Activity(mA/cm ²)	Reference
Pt ₇₅ Pd ₂₅ /rGO-CNTs	0.5 M H ₂ SO ₄ +1 M CH ₃ OH	1.01	5.4	1
Pt ₆₀ Pd ₄₀ -GNP	0.5 M H ₂ SO ₄ +1 M CH ₃ OH	0.47	0.263	2
PtPdCu-TiN	0.5M H ₂ SO ₄ +0.5M CH ₃ OH	0.37	0.48	3
PtPd-TiN	0.5 M H ₂ SO ₄ +0.5 CH ₃ OH	0.2	0.27	4
Pt ₃ Pd ₁ -CeO ₂ /C	0.5 M HClO ₄ +1 M CH ₃ OH	0.853	2.05	5
Pt₆₂Pd₃₈/C	0.1M HClO ₄ +0.5 M CH ₃ OH	1.31	0.57	This work

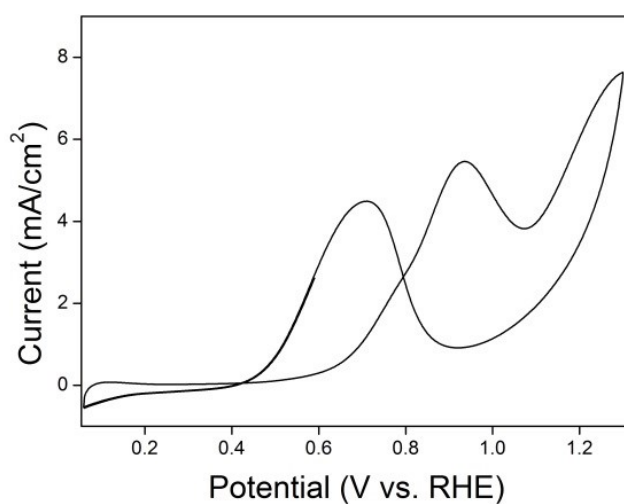


Fig. S4 CV curves of commercial Pt/C in 0.1 M HClO₄ + 0.5 M C₂H₅OH solution purged with N₂ at a scan rate of 50 mV s⁻¹

Table S2 Comparison of MOR activities of various catalysts

Catalyst	Electrolyte	Mass activity (A/mg_{Pt}^{-1})	Specific activity(mA/cm^2)	Reference
Pt ₇₃ Pd ₂₇ /C	0.5 M H ₂ SO ₄ +1 M C ₂ H ₅ OH	0.482	0.54	6
PtPd NPs	0.5 MH ₂ SO ₄ +0.5MC ₂ H ₅ OH	0.49	1.12	7
Pt ₃₄ Pd ₃₃ Cu ₃₃	0.1M HClO ₄ +0.5MC ₂ H ₅ OH	0.19	1.13	8
Pt ₁ Pd ₅ NC/RGO	0.5 M H ₂ SO ₄ +0.5MC ₂ H ₅ OH	1.08	2.31	9
Pt-Pd@TDI/rGO	0.1MHClO ₄ +0.5MC ₂ H ₅ OH	1.5	1.20	10
Pt₆₂Pd₃₈/C	0.1M HClO ₄ +0.5MC ₂ H ₅ OH	1.2	0.87	This work

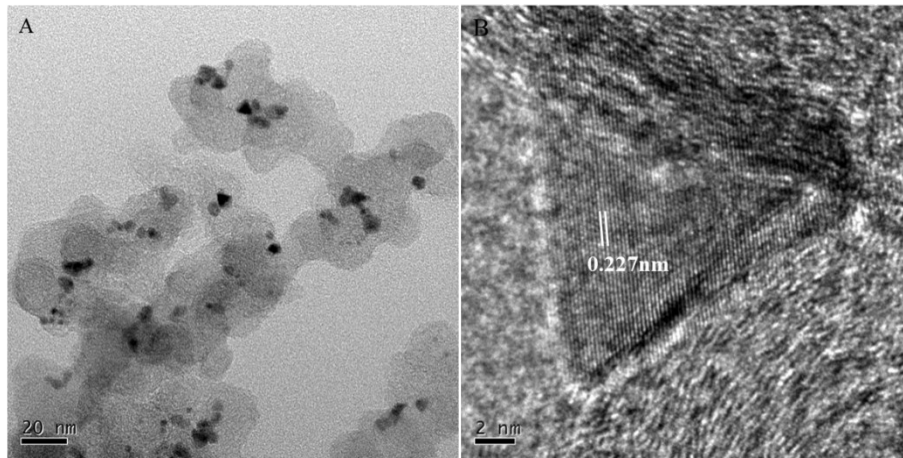








Fig. S5 TEM images of Pt₆₂Pd₃₈/C alloy NTDs after long-term durability

Table S3. Structure, binding energy (E_{binding}) and d-band center for Pt_nPd_{10-n} clusters

	Cluster	E_{binding} (eV)	d-band center (eV)
Pt ₁₀		1.461	-1.125
Pt ₈ Pd ₂		1.464	-1.048
Pt ₆ Pd ₄		1.466	-0.856
Pt ₃ Pd ₇		1.465	-0.801
Pt ₁ Pd ₉		1.463	-0.365
Pd ₁₀		1.462	-0.253

Reference

- 1 A. B. Yousaf, M. Imran, S. J. Zaidi and P. Kasak, *J. Electroanal. Chem.*, 2019, **832**, 343-352.
- 2 G. L. Zhang, C. D. Huang, R. J. Qin, Z. C. Shao, D. An, W. Zhang and Y. X. Wang, *J. Mater. Chem. A*, 2015, **3**, 5204-5211.
- 3 R. Chang, L. J. Zheng, C. W. Wang, D. C. Yang, G. X. Zhang and S. H. Sun, *Appl. Catal. B: Environ.*, 2017, **211**, 205-211.
- 4 M. X. Gong, X. Jiang, T. Y. Xue, T. Y. Shen, L. Xu, D. M. Sun and Y. W. Tang, *Catal. Sci. Technol.*, 2013, **00**, 1-3.
- 5 A. B. Yousaf, M. Imran, N. Uwitonze, A. Zeb, S. J. Zaidi, T. M. Ansari, G. Yasmeen and S. Manzoor, *J. Phys. Chem. C*, 2017, **121**, 2069-2079.
- 6 Q. Zhang, T. Chen, R. Y. Jiang and F. X. Jiang, *RSC Adv.*, 2020, **10**, 10134-10143.
- 7 P. T. Qiu, S. M. Lian, G. Yang and S. C. Yang, *Nano Rev.*, 2017, **10**, 1064-77.
- 8 J. Lan, K. Wang, Q. Yuan and X. Wang, *Mater. Chem. Front.*, 2017, **1**, 1217-22.
- 9 Y. Y. Zheng, J. H. Qiao, J. H. Yuan, J. F. Shen, A. J. Wang and S. T. Huang, *Inter. J. Hydrogen Energ.*, 2018, **43**, 4902-4911.
- 10 J. N. Tiwari, W. G. Lee, S. Sultan, M. Yousuf, A. M. Harzandi, V. Vij and K. S. Kim, *ACS Nano.*, 2017, **11**, 7729-7735.