

Supporting Information

Synergism of Pt single atoms, clusters and nanoparticles on carbon doping with nitrogen for nitroaromatics highly efficient and selective hydrogenation

Yu Fang^{a,1}, Qingqing Liu^{a,1}, Min Tian^{b,1}, Luna Ruan^{a,1}, Kai Chen^a, Huan Zhang^a, Zhiqing Yang^{b,*}, Hengqiang Ye^b, Lihua Zhu^{a,*}

^a Jiangxi Province Key Laboratory of Functional Crystalline Materials Chemistry, College of Chemistry and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, Jiangxi, China.

^b Ji Hua Laboratory, Foshan 528200, PR China

¹ These authors contributed equally to this work.

Corresponding authors.

E-mail addresses: yangzq34@163.com (Zhiqing Yang); zhulihua@jxust.edu.cn (Lihua Zhu)

Table S1. Specific surface area, pore volume and average pore size of different samples.

Catalyst	BET surface area (m ² ·g ⁻¹)	Average pore diameter (nm)	Total pore volume (cm ³ ·g ⁻¹)
NC	1515.9	2.44	74.3
1.08%Pt/NC	1426.2	2.24	70.9

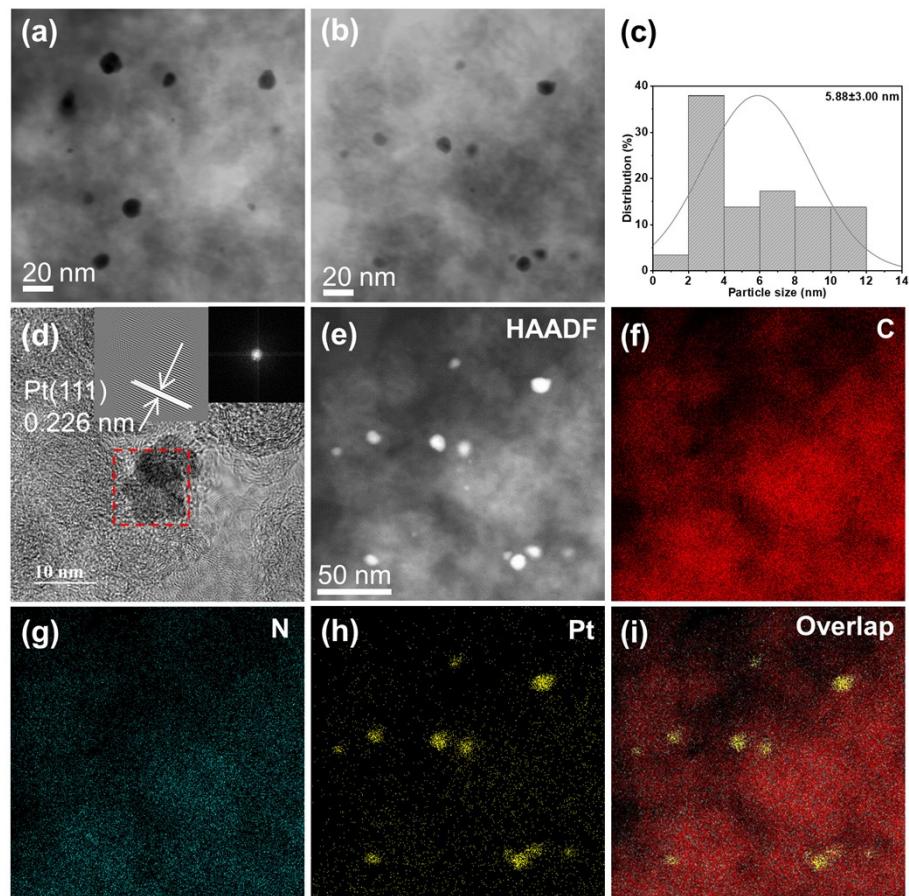


Fig. S1. (a, b) TEM images, (c) particle size distribution of 1.08% Pt/NC, (d) HRTEM image, (e) HADDF-STEM image, (f-i) STEM-EDS elemental mapping of 1.08% Pt/NC (red: C, blue: N, yellow: Pt, elements overlaid).

Table S2. The catalytic performance of the reported catalysts for nitrobenzene hydrogenation in the literature.

Ref. ^[a]	Catalyst	Substrate	Solvent	T (°C)	Time (h)	H ₂ Pressure (MPa)	TOF (h ⁻¹)	S ^[b] (%)	Y ^[c] (%)
[1]	Co ₁ @NC-(SBA)	nitrobenzene	ethanol	90	1.5	1.0	-	99%	99%
[2]	Ru@C ₆₀	nitrobenzene	isopropanol	80	6	3.0	37	100%	100%
[3]	Pt/H-NCNTs	nitrobenzene	ethylbenzene	40	0.33	0.5	11358	99%	97%
[4]	Pd/MIL-101	nitrobenzene	DMF	120	6	0.6	-	>99.9%	>99.9%
[5]	Co/NC-0.30	nitrobenzene	ethanol	70	4	3.0	-	>99%	>99%
[6]	2.5%Pd/CeO ₂	nitrobenzene	solvent-free	40	3	6.0	11411	100%	100%
[7]	Pd-6Ni-N-C ₆₀	nitrobenzene	ethanol	80	0.33	1.0	-	99.8%	98.5%
[8]	Pt/Ti ₃ C ₂ T _x -D-AB	nitrobenzene	ethanol/water	30	1	1.0	-	100%	99.2%
[9]	Pd@P(QP-TVP)	nitrobenzene	H ₂ O	40	1	1.0	-	100%	98.6%
[10]	Pd@HTMC	nitrobenzene	H ₂ O	50	1	0.1	-	100%	100%
[11]	Co@NMC-800	nitrobenzene	ethanol	80	1.33	1.0	364.9	>99%	>98%
[12]	Fe ₂ O ₃ @G-C-900	nitrobenzene	ethanol	70	2	2.0	-	99.1%	94.5%
[13]	Ni@C-650	nitrobenzene	ethanol	140	0.66	0.5	-	98.7%	97.7%
This work	1.08% Pt/NC	nitrobenzene	ethanol	30	0.05	1.0	74191.8	97.7%	98.9%

[a] Reference; [b] Selectivity to the target product of only -NO₂ group hydrogenation; [c] Yield to the target product of only -NO₂ group hydrogenation.

References

- [1] L. Zhang, N. Shang, S. Gao, J. Wang, T. Meng, C. Du, T. Shen, J. Huang, Q. Wu, H. Wang, Y. Qiao, C. Wang, Y. Gao and Z. Wang, *ACS Catal.*, 2020, **10**, 8672–8682.
- [2] F. Leng, I. C. Gerber, P. Lecante, S. Moldovan, M. Girleanu, M. R. Axet and P. Serp, *ACS Catal.*, 2016, **6**, 6018–6024.
- [3] W. Shi, B. Zhang, Y. Lin, Q. Wang, Q. Zhang and D. S. Su, *ACS Catal.*, 2016, **6**, 7844–7854.
- [4] X. Chen, K. Shen, D. Ding, J. Chen, T. Fan, R. Wu and Y. Li, *ACS Catal.*, 2018, **8**, 10641–10648.
- [5] Y. Dai, C. Jiang, M. Xu, B. Bian, D. Lu and Y. Yang, *Appl. Catal. A-Gen.*, 2019, **580**, 158–166.
- [6] X. Shi, X. Wang, X. Shang, X. Zou, W. Ding and X. Lu, *ChemCatChem*, 2017, **9**, 3743–3751.
- [7] Y. Qu, T. Chen and G. Wang, *Appl. Surf. Sci.*, 2019, **465**, 888–894.
- [8] Q. Chen, W. Jiang and G. Fan, *Dalton Trans.*, 2020, **49**, 14914–14920.
- [9] Y. Lei, Z. Chen, G. Lan, R. Wang and X.-Y. Zhou, *New J. Chem.*, 2020, **44**, 3681–3689.
- [10] S. Sadjadi, M. Akbari, E. Monflier, M. M. Heravi and B. Leger, *New J. Chem.*, 2018, **42**, 15733–15742.
- [11] F. Zhang, C. Zhao, S. Chen, H. Li, H. Yang and X.-M. Zhang, *J. Catal.*, 2017, **348**, 212–222.
- [12] Y. Wang, J. Shi, Z. Zhang, J. Fu, X. Lü and Z. Hou, *Chin. J. Catal.*, 2017, **38**, 1909–1917.
- [13] B. Tang, W.-C. Song, E.-C. Yang and X.-J. Zhao, *RSC Adv.*, 2017, **7**, 1531–1539.