

Synthesis and Catalytic Activity of Palladium Supported on Heteroatom Doped Single-wall Carbon Nanohorns

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

www.rsc.org/

Xueyou Tan,^a Xiaohui Wu,^a Ziqi Hu,^a Ding Ma^b and Zujin Shi*^a

^a Beijing National Laboratory for Molecular Sciences, State Key Lab of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China.
E-mail: zjshi@pku.edu.cn

^b Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China.

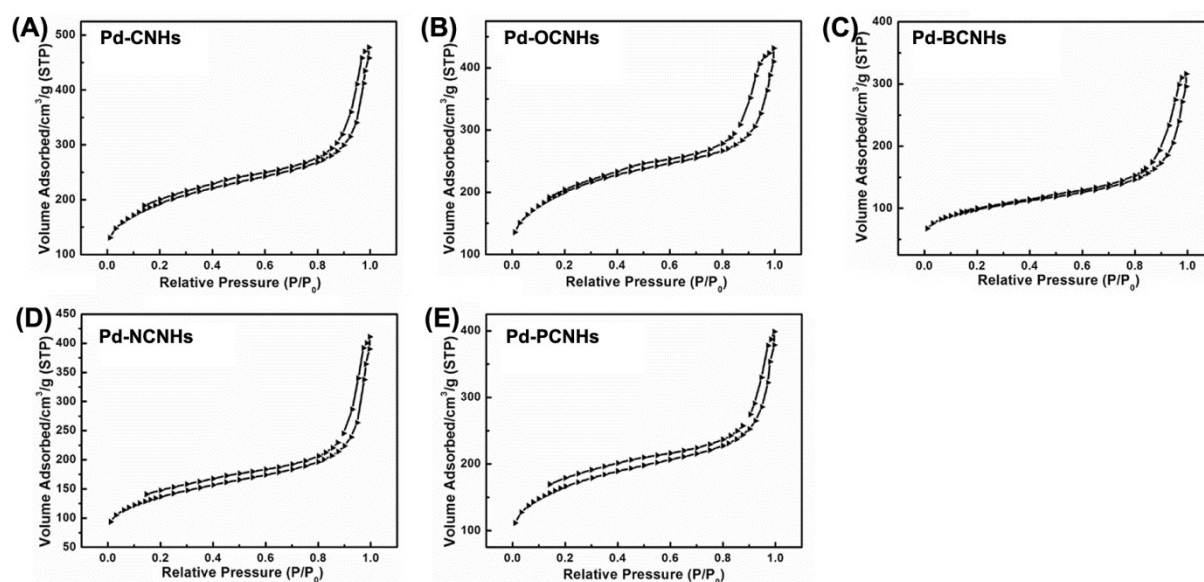


Fig. S1 N₂ adsorption-desorption isotherms of (A) Pd-CNHs, (B) Pd-OCNHs, (C) Pd-BCNHs, (D) Pd-NCNHs and (E) Pd-PCNHs, respectively.

Table S1 BET specific surface area (m² g⁻¹) and pore size (nm) of catalysts

	BET specific surface area (m ² g ⁻¹)	Pore size (nm)
Pd-CNHs	672.5	3.74
Pd-OCNHs	697.4	3.17
Pd-BCNHs	355.7	4.30
Pd-NCNHs	475.4	4.35
Pd-PCNHs	578.9	3.40

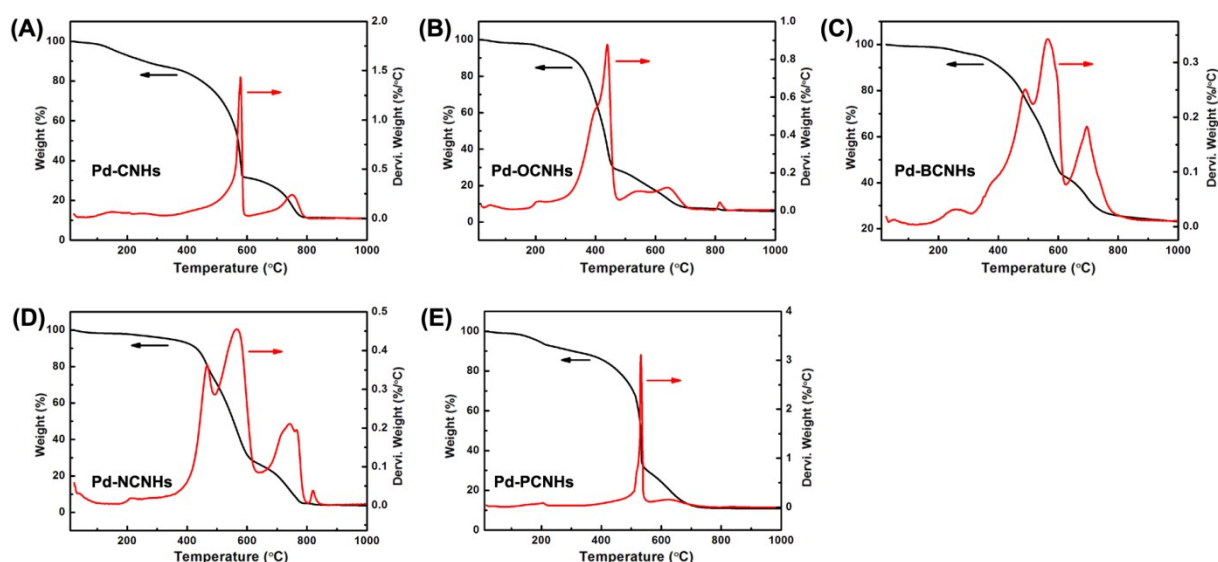


Fig. S2 TGA curves of (A) Pd-CNHS, (B) Pd-OCNHS, (C) Pd-BCNHS, (D) Pd-NCNHS, and (E) Pd-PCNHS, respectively.

For Pd-CNHS, the peaks at 579.5 and 749.8 °C were described as CNHS and graphitic carbon,¹⁻² respectively. The peaks at 439, 643 and 815 °C in the Pd-OCNHS were attributed to combination of defective carbon, tubular graphene carbon and graphitic carbon, respectively. For Pd-BCNHS, graphitic carbon, B-doped CNHS and tubular graphene carbon can be burned at 489, 564 and 695 °C.¹⁻² Pd-NCNHS shows two main peaks at 467 °C and 565 °C, separately, which were attributed to a combination of N-doped defective carbon and N-doped tubular graphene carbon, and two peaks at 743 °C and 766 °C were both ascribed to graphitic carbon. For Pd-PCNHS, a main peak at 532 °C and a concomitantly weak peak at 634 °C appeared, corresponding to P-doped defective carbon and tubular graphene carbon, respectively.

Table S2 The atomic percent of dopants in sample determined by XPS

Sample	C (At%)	O (At%)	B (At%)	N (At%)	P (At%)
Pd-CNHS	98.79	1.09	0	0	0
Pd-OCNHS	97.50	2.33	0	0	0
Pd-BCNHS	96.37	2.72	0.71	0	0
Pd-NCNHS	97.44	1.06	0	1.33	0
Pd-PCNHS	98.39	1.39	0	0	0.07

Table S3 The proportion of surface palladium species in sample determined by XPS

Sample	Pd ⁰ (%)	Pd ²⁺ (%)
Pd-CNHS	32.95	67.05
Pd-OCNHS	61.73	38.27
Pd-BCNHS	60.88	39.12
Pd-NCNHS	32.54	67.46
Pd-PCNHS	33.51	66.49

Notes and references

1 X. Wu, L. Cui, P. Tang, Z. Hu, D. Ma and Z. Shi, *Chem. Commun.*, 2016, **52**, 5391.

2 L. Sun, C. Wang, Y. Zhou, X. Zhang, B. Cai and J. Qiu, *Appl. Surf. Sci.*, 2013, **277**, 88.