Supporting Information

Pd/N, S co-doped activated carbon as a highly-efficient catalyst for the one-pot synthesis of meropenem

Yuefeng Li,[a, b,c] Fengmei Xiong,[d] Jiangmei Yan,[b,c] Zhaowen Wang,[b,c] Tao Hong,[a] Zhixiang Zhang,[b,c] Yu Li[a]* and Xinli Jing[a]*

[a] *School of Chemistry, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, P. R. China;*

[b] *Department of Technology, Kaili Catalyst & New Materials Co., Ltd., Xi'an, Shaanxi, 710201, P. R. China;*

[c] *Shaanxi Key Laboratory of Catalytic Materials and Technology, Xi'an, Shaanxi, 710201, P. R. China*

[d] *Department of Pharmacy, Xi'an Children's Hospital, Xi'an, Shaanxi, 710004, P. R. China.*

* *Corresponding authors:*

Email: xljing@mail.xjtu.edu.cn, yuli2012@mail.xjtu.edu.cn

6 pages, 5 figures, 4 tables

Contents

S6

Analysis of impurities in meropenem

Based on the analysis method, [32,49] the contents of impurities were determined via high-performance liquid chromatography (Shimadzu Prominence LC-20A). Chromatography was performed on a Shim-pack CLC-ODS C18 (150 mm × 4.6 mm, 5 μm) analytical column with 0.1% triethylamine solution–acetonitrile (100:7) as the mobile phase. The column was maintained at a constant temperature of 40°. The flow rate was about 1.6 $mL \cdot min^{-1}$, and the ultraviolet (UV) detection wavelength was 220 nm. Here, the triethylamine solution was prepared by adding 900 mL of distilled water to 1.0 mL of triethylamine; the solution was adjusted with diluted phosphoric acid to a pH of 5.0 ± 0.1, then diluted with water to 1000 mL. Crude meropenem (0.05 g) was dissolved in a 0.1% triethylamine solution to obtain the test solution, 10 μL of which was injected for chromatography, and the chromatogram was recorded.

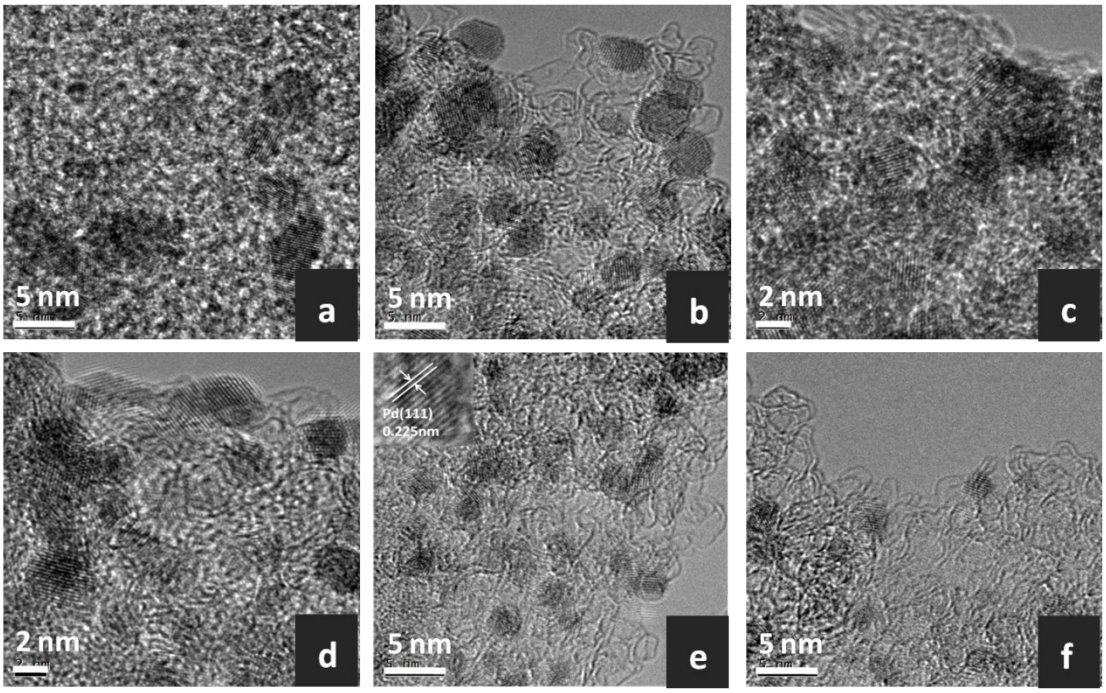

Fig. S1 The high-resolution TEM images of the Pd/C catalysts: (a) Pd/C0, (b) Pd/C1, (c) Pd/C2, (d) Pd/C3, (e) Pd/C4, and (f) Pd/C5.

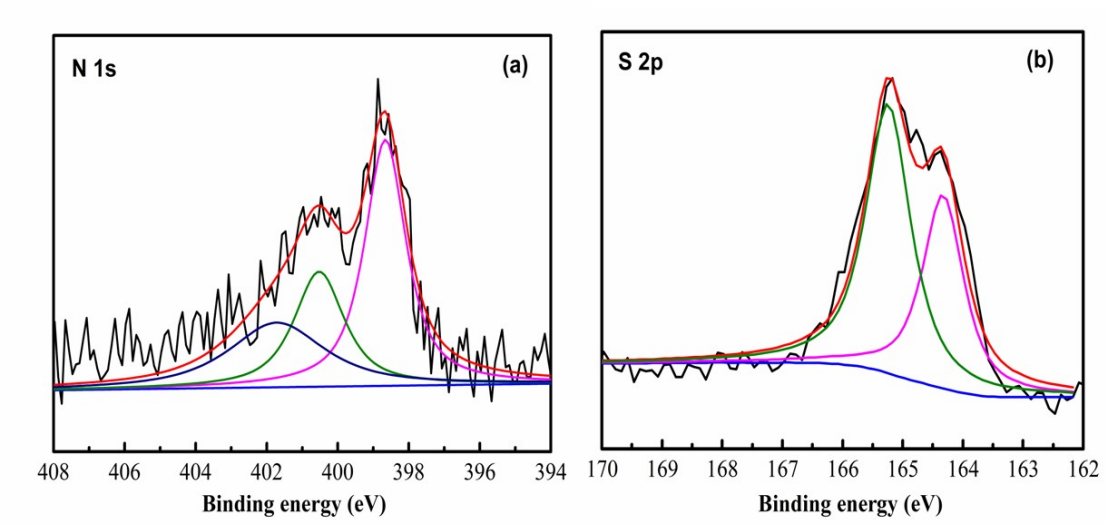

Fig. S2 N 1s and S 2p XPS spectra of the C1-2N (a) and C5-0N (b) samples

Table S1 N 1s and S 2p XPS spectral line fitting for the C1-2N and C5-0N samples

AC	Mass fraction of N (%)	Mass fraction of S (%)	Relative atomic percentage (%)				
			N (398.5eV)	N (400.1eV)	N (401.2eV)	S (164.1eV)	S (165.2eV)
C1-2N	2.53	0	46.08	26.09	27.83	-	-
C5-0N	0	0.52	-	-	-	39.79	60.21

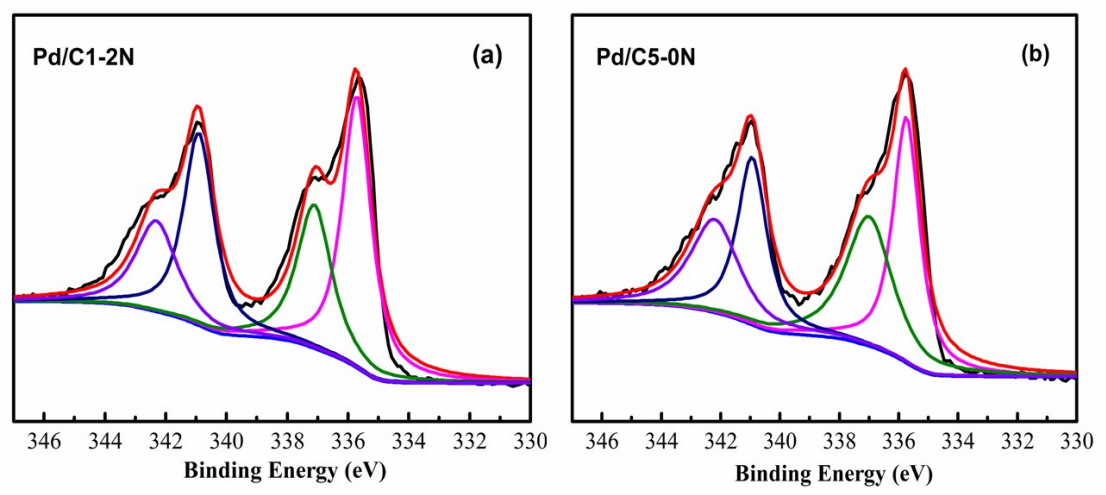

Fig. S3 XPS spectra of the Pd/C1-2N (a) and Pd/C5-0N (b) catalyst.

Table S2 XPS spectral line fitting for the Pd/C1-2N and Pd/C5-0N catalyst

Catalyst	Pd^0 (%)	Pd^{2+} (%)
Pd/C1-2N	61.31	38.69
Pd/C5-0N	52.46	47.54

Table S3 Meropenem yield under different Pd/C catalysts under the repeat experiments

Entry	Yield of meropenem* (%)			
	Pd/C2	Pd/C3	Pd/C4	Pd/C5
1	48.52	49.25	50.33	49.70
2	48.60	49.30	50.43	49.74
3	48.68	49.36	50.48	49.78
4	48.61	49.39	50.52	49.85
5	48.73	49.43	50.48	49.65
Average value (%)	48.628	49.346	50.448	49.744
Standard deviation (%)	0.080	0.072	0.073	0.076

* Yield of meropenem: reaction under 0.15 g of the side chain

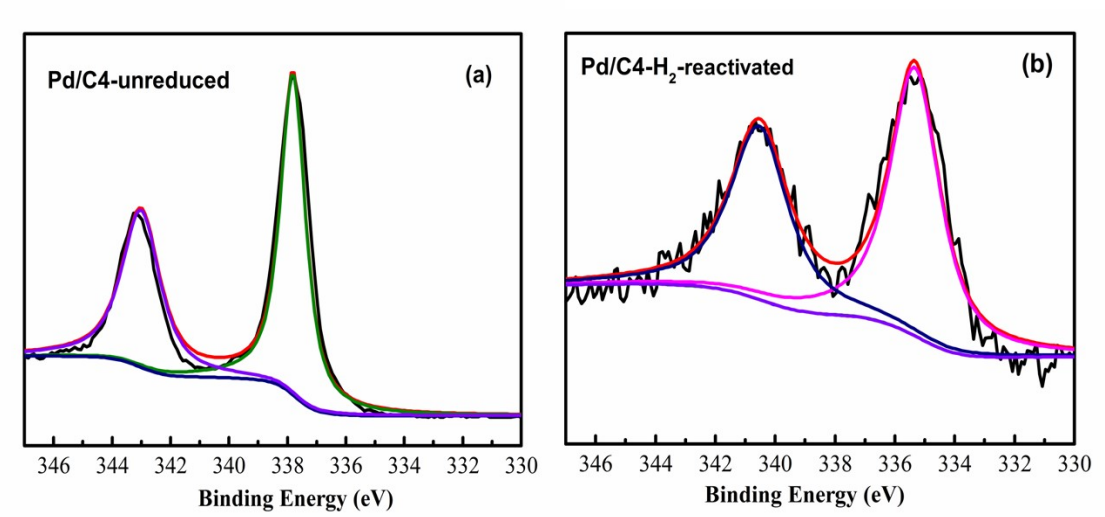

Fig. S4 XPS spectra of the Pd/C4-unreduced (a) and Pd/C4-H_2-reactivated (b) catalyst.

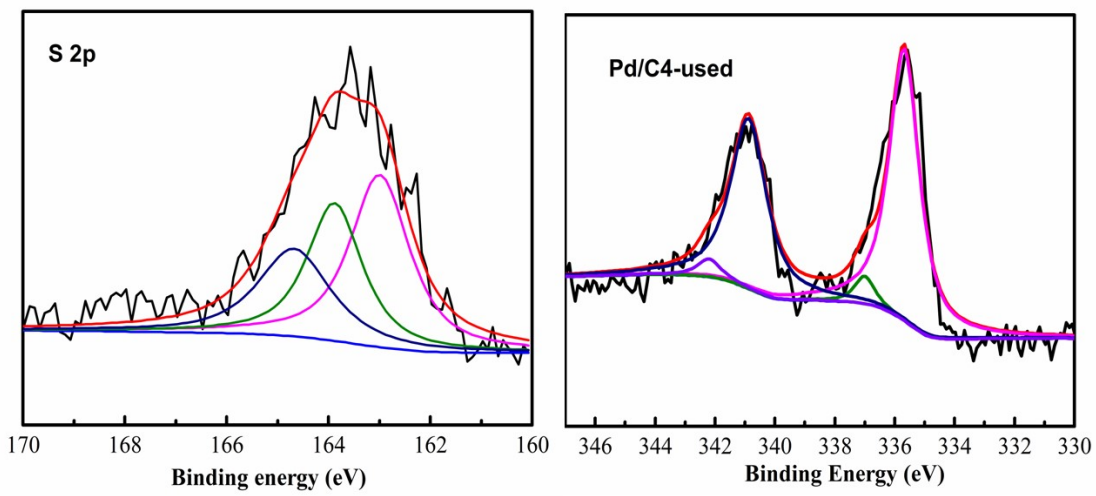

Fig. S5 S 2p and Pd 3d XPS spectra of the Pd/C4-used catalyst

Table S4 Impurity contents, Pd content, and color of meropenem products obtained over different Pd/C catalysts

Sample*	Color	Ring-opening compound (%)	Dimers (%)	Total impurity content (%)	Pd content (ppm)
Pd/C2	White	0.11	0.13	0.63	7
Pd/C3	White	0.13	0.14	0.61	7
Pd/C4	White	0.10	0.11	0.60	6
Pd/C5	White	0.12	0.12	0.60	7
Pd/C1-2N	White	0.18	0.16	0.65	8
Pd/C5-0N	White	0.16	0.17	0.68	7
Pd/C4-unreduced	White	0.13	0.13	0.64	8
Pd/C4-H_2-reactivated	White	0.12	0.15	0.69	6

* meropenem product: reaction under 0.15 g of the side chain