

# Significantly Enhanced Catalytic Performance of Pd Nanocatalyst on AlOOH Featuring Abundant Solid Surface Frustrated Lewis Pair for Improved Hydrogen Activation

Junwei Li,<sup>a</sup> Hongshuai Yin,<sup>a</sup> Sisi Liu,<sup>a</sup> Chaofa Xu,<sup>\*a,b</sup> and Zhixiong Cai<sup>\*a,b</sup>

<sup>a</sup> College of Chemistry, Chemical Engineering and Environment, Minnan Normal University, Zhangzhou, China

<sup>b</sup> Fujian Provincial Key Laboratory of Modern Separation and Analysis Science and Technology, Zhangzhou, China

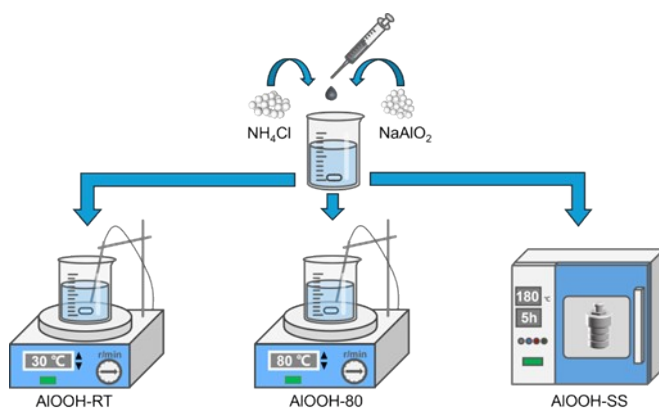


Figure S1. Schematic of the synthesis of AlOOH with different crystallinities.

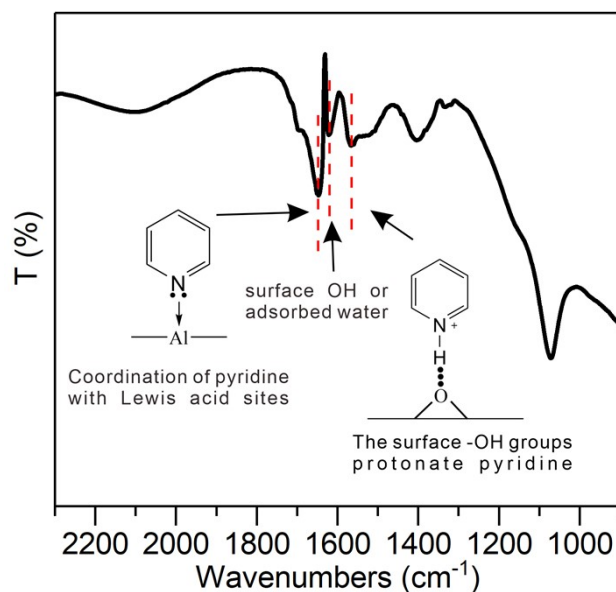


Figure S2. FT-IR spectra of pyridine adsorption on AlOOH-80. The absorption peak at 1647 cm<sup>-1</sup> corresponded to the coordination of pyridine molecules with unsaturated Al sites (Lewis acid sites) exposed on the surface. The absorption peak at 1615 cm<sup>-1</sup> was attributed to surface hydroxyl groups or adsorbed water, while at 1567 cm<sup>-1</sup>, protonation of pyridine by the surface -OH groups was indicated.

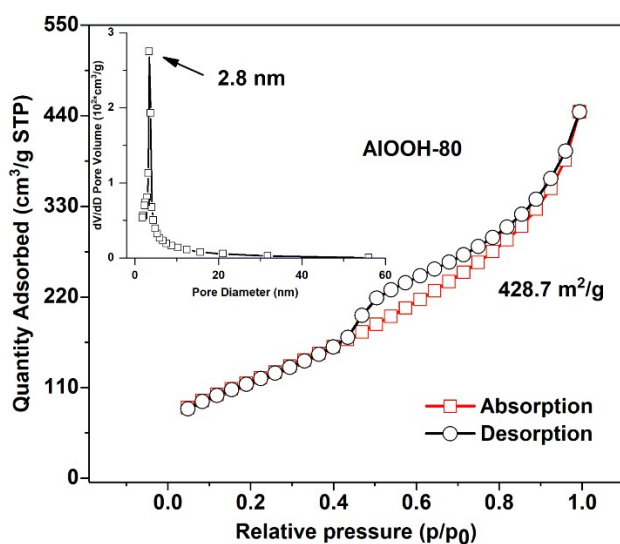


Figure S3. N<sub>2</sub> adsorption-desorption isotherms and pore diameter distribution curve of AlOOH-80.

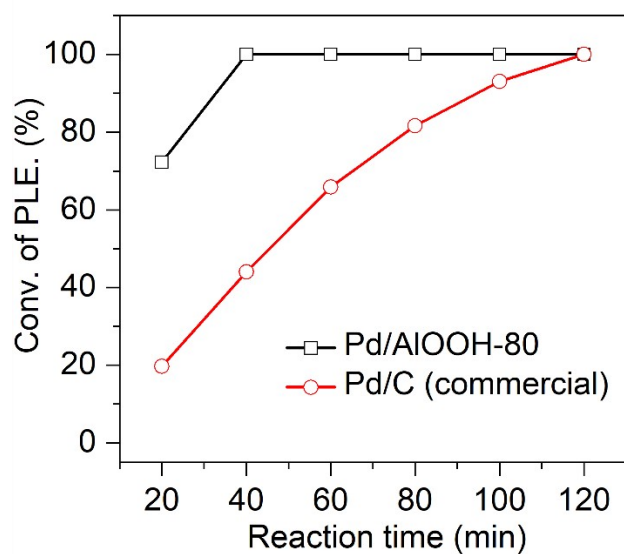


Figure S4. Pd/AlOOH-80 compared with commercial palladium on C (Pd/C) for catalytic performance.

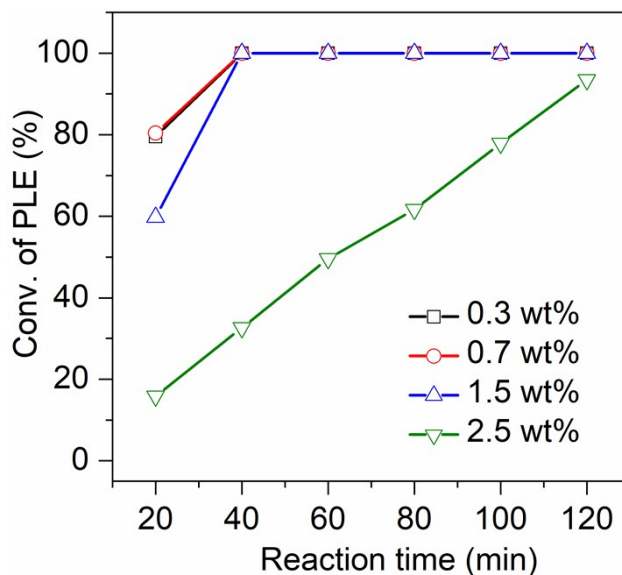


Figure S5. Catalytic performance of hydrogenation of phenylacetylene on Pd/AlOOH-80 with different Pd loadings.

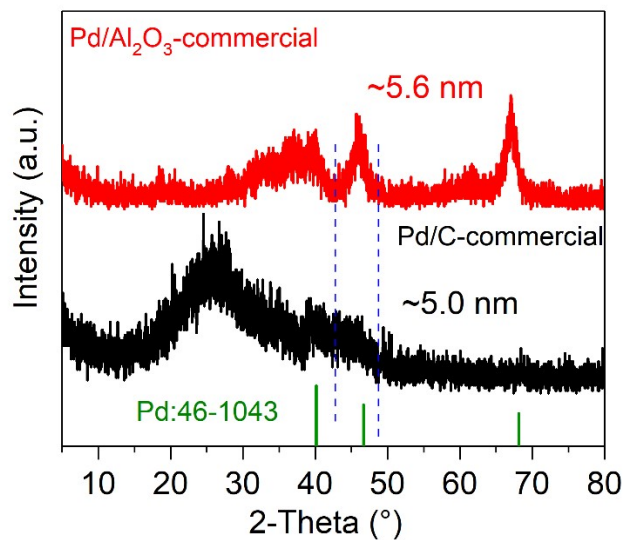


Figure S6. XRD patterns of commercial Pd/Al<sub>2</sub>O<sub>3</sub> and commercial Pd/C. The average size of nanoparticles was calculated using the Scherrer equation based on the half-width of peaks.

Table S1. Results of XPS analysis of O1s of the AlOOH catalysts

Entry	Catalyst	O <sub>adH2O</sub> /O <sub>Total</sub> (%)
1	AlOOH-80	8.7
2	AlOOH-RT	17.2
3	AlOOH-SS	22.5

Table S2. The Pd content in Pd/AlOOH-80 catalyst was measured by ICP-AES.

Entry	Catalyst	Theoretical load (wt%)	Actual load (wt%)
1	AlOOH-80	0.3	0.4
2	AlOOH-80	0.7	0.7
3	AlOOH-80	1.5	1.7
4	AlOOH-80	2.5	2.2

Table S3. Catalytic performance comparison between Pd/AlOOH-80 and previously reported catalysts of the hydrogenation of phenylacetylene.

Entry	Catalyst	T (°C)	Hydrogen source	Time	Con. (%)	Reaction rate (h <sup>-1</sup> )	Ref.
1	Pd <sub>2</sub> Cu <sub>2</sub> @ $\alpha$ -Al <sub>2</sub> O <sub>3</sub>	30	0.1 MPa H <sub>2</sub>	70 min	>99.9	146.2	1
2	Pd <sub>1</sub> /NC-PHF	60	0.5 MPa H <sub>2</sub>	2 h	93.1	88.5	2
3	Pd <sub>1</sub> /BP	80	2 bar H <sub>2</sub>	4 h	95	133.0	3
4	Pd <sub>4,5</sub> Se NCs/C	110	0.1 MPa H <sub>2</sub>	1.5 h	100	358.6	4
5	PdCu <sub>2</sub> @MF-H	30	0.1 MPa H <sub>2</sub>	4 h	100	125.9	5
6	PdCu@Cu <sub>2</sub> O	30	0.1 MPa H <sub>2</sub>	80 min	>99	1500.0	6
7	Pd <sub>1</sub> /Cu <sub>2</sub> O	30	0.1 MPa H <sub>2</sub>	60 min	100	500.0	7
8	Pd/AlOOH-80	30	0.1 MPa H <sub>2</sub>	40 min	100	4500.0	This work

$$\text{Reaction rate} = \frac{\text{moles of phenylacetylene}}{\text{moles of Pd} \times \text{reaction time (h)}}$$

## References

1. J. Li, W. Suo, Y. Huang, M. Chen, H. Ma, C. Liu, H. Zhang, K. Liang, Z. J. J. o. C. Dong and I. Science, 2023, **652**, 1053-1062.
2. S. Li, G. Yue, H. Li, J. Liu, L. Hou, N. Wang, C. Cao, Z. Cui and Y. J. C. E. J. Zhao, 2023, **454**, 140031.
3. C. Chen, W. Ou, K. M. Yam, S. Xi, X. Zhao, S. Chen, J. Li, P. Lyu, L. Ma and Y. J. A. M. Du, 2021, **33**, 2008471.
4. M. Wang, L. Liang, X. Liu, Q. Sun, M. Guo, S. Bai and Y. J. J. o. C. Xu, 2023, **418**, 247-255.
5. M. Guo, Q. Meng, W. Chen, Z. Meng, M. L. Gao, Q. Li, X. Duan and H. L. J. A. C. Jiang, 2023, **135**, e202305212.
6. K. Liu, L. Jiang, W. Huang, G. Zhu, Y.-J. Zhang, C. Xu, R. Qin, P. Liu, C. Hu and J. J. N. C. Wang, 2022, **13**, 2597.
7. K. Liu, R. Qin, L. Zhou, P. Liu, Q. Zhang, W. Jing, P. Ruan, L. Gu, G. Fu and N. J. C. C. Zheng, 2019, 207-214.