

Supporting Information

Monolithic Wood-Based Carbon Supported Pd Nanoparticles with Tunable Exposure for Boosting Semi-Hydrogenation of Alkynols

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Supplementary Figures and Tables

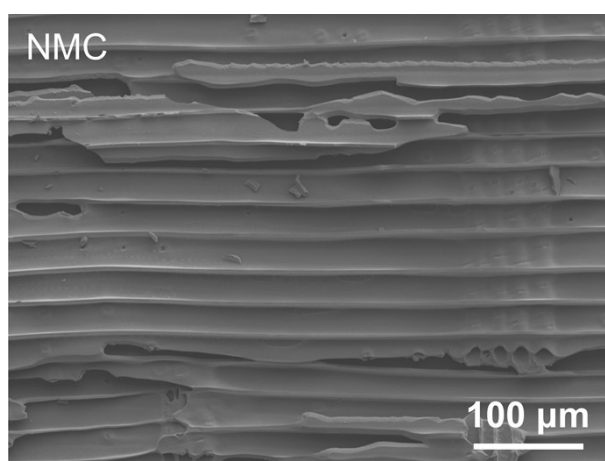


Fig. S1 SEM image of NMC along the parallel growth direction of the wood.

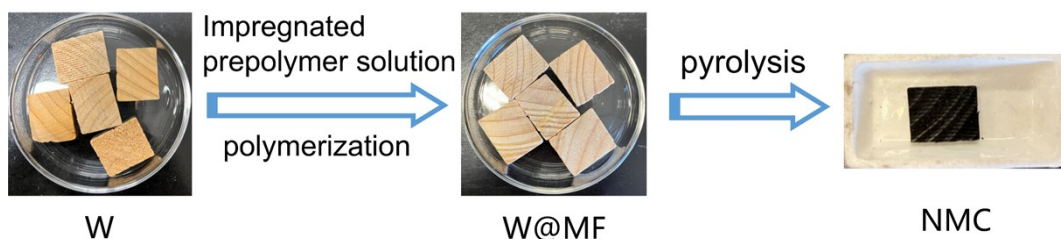


Fig. S2 Photographs of W, W@MF, and NMC.

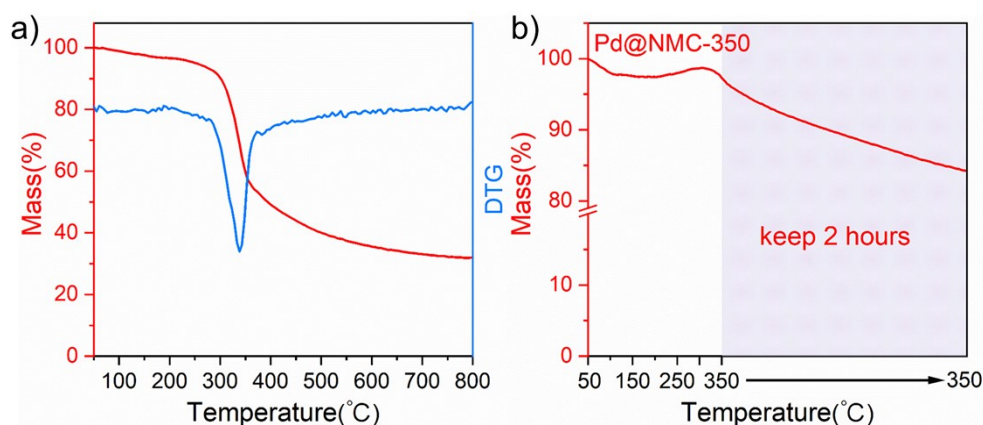


Fig. S3 a) TG and DTG curves of the W@MF heated from ambient temperature to 800 °C at a rate of 10°C min⁻¹ under N₂ flow. b) The TG curve of the NMC heated from ambient temperature to 350 °C staying for 2 h at a rate of 10°C min⁻¹ under the Air flow.

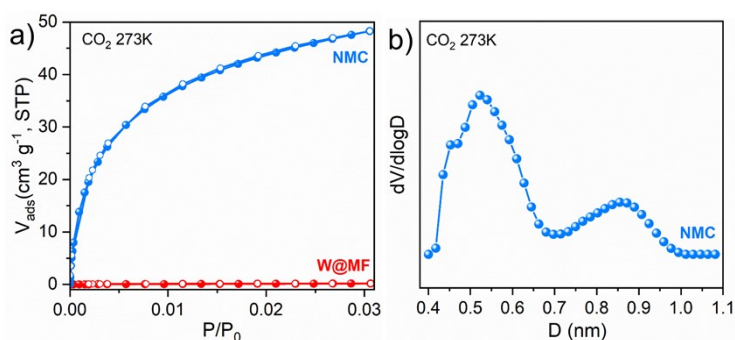


Fig. S4 a) CO₂ adsorption-desorption isotherms of W@MF and NMC at 273 K.

b) Pore size distribution of NMC determined from CO₂ adsorption at 273 K.

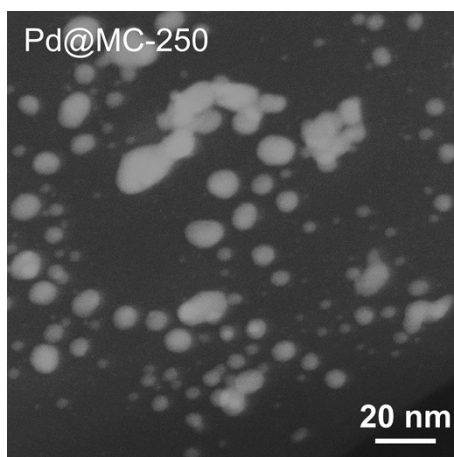


Fig. S5 STEM image of the Pd@MC-250 catalyst.

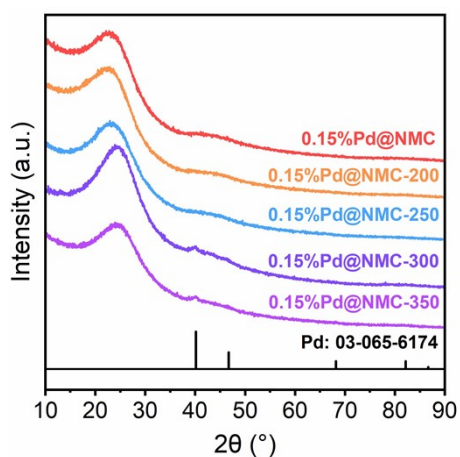


Fig. S6 XRD patterns of the different monolithic carbon catalysts.

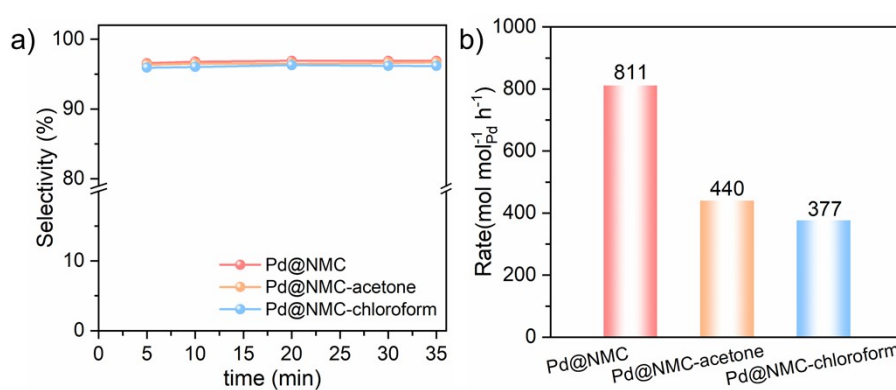


Fig. S7 a) Selectivity of MBE upon Pd@NMC, Pd@NMC-acetone and Pd@NMC-chloroform. b) Reaction rates of the catalysts.

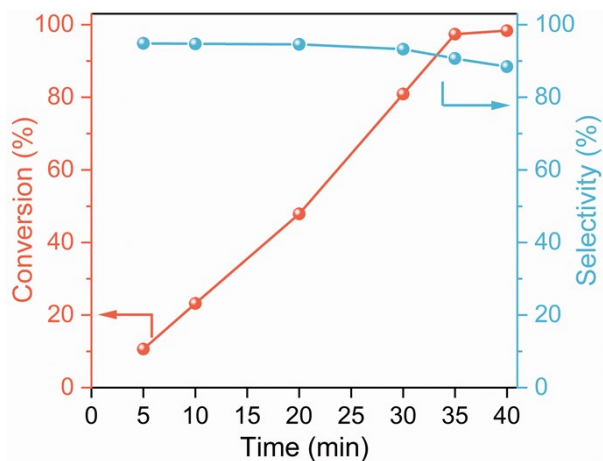


Fig. S8 Conversion of MBY and selectivity of MBE upon Pd@NMC-250.

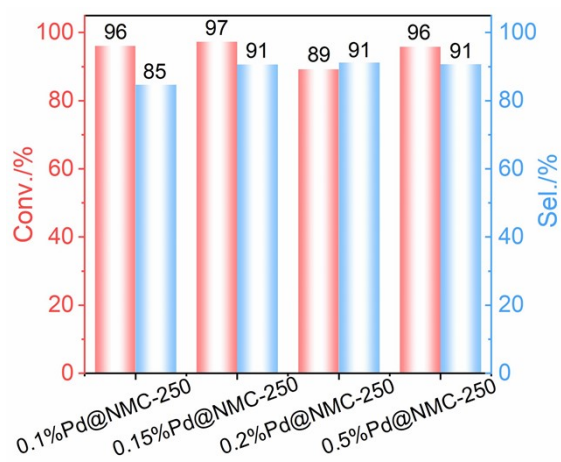


Fig. S9 Conversion of MBY and selectivity of MBE upon catalysts with different metal loadings.

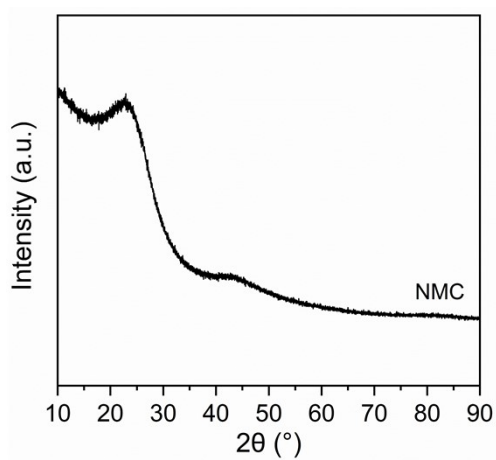


Fig.S10 XRD patterns of the N-doped monolithic carbon (NMC).

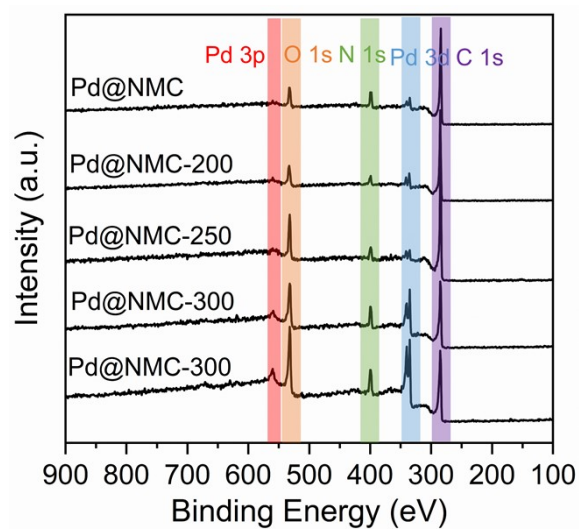


Fig.S11 XPS spectrum of different monolithic carbon catalysts.

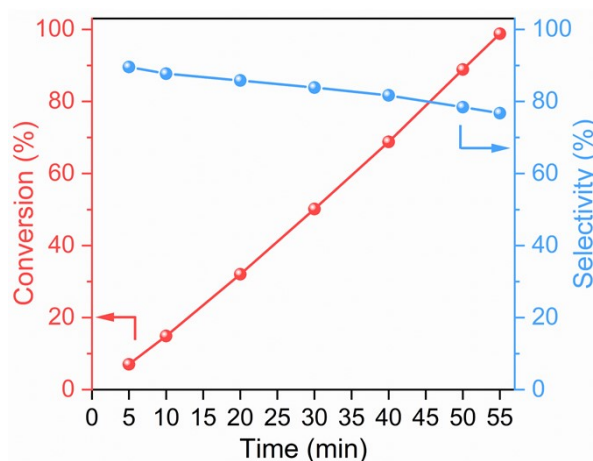


Fig. S12 Conversion of MBY and selectivity of MBE upon Pd@MC-250.

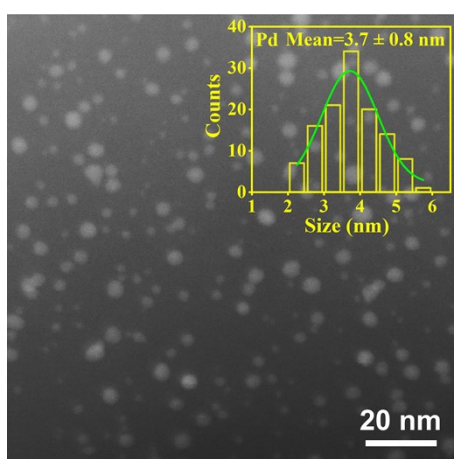


Fig. S13 STEM image and particle size distribution of the Pd@NMC-250

(The catalyst after five cycles of reaction).

Table S1 Surface atomic ratio obtained from X-ray photoelectron spectroscopy.

Sample	C (%)	N (%)	O (%)	Pd (%)
Pd@NMC	79.12	10.93	9.29	0.66
Pd@NMC-200	79.20	8.22	11.64	0.94
Pd@NMC-250	76.50	6.92	15.03	1.55
Pd@NMC-300	63.38	12.33	21.45	2.84
Pd@NMC-350	56.76	12.76	26.70	3.78

Table S2 ICP-OES of the different monolithic carbon catalysts.

Entry	Catalysts	Theoretical Pd loading/wt.%	Actual Pd loading/wt.%
1 ^[a]	Pd@NMC	0.150	0.133
2 ^[a]	Pd@NMC-200	0.150	0.137
3 ^[a]	Pd@NMC-250	0.150	0.138
4 ^[b]	Pd@NMC-250	0.150	0.135
5 ^[a]	Pd@NMC-300	0.150	0.132
6 ^[b]	Pd@NMC-300	0.150	0.114
7 ^[a]	Pd@NMC-350	0.150	0.139

[a] As-prepared fresh catalysts; [b] The catalysts after five cycles.

Table S3 Catalytic performance in the 2-methyl-3-butyn-2-ol hydrogenation reaction over various catalysts.

Catalysts	Conv. (%)	Sel. (%)	Rate (mol mol _{cat} ⁻¹ h ⁻¹)	Conditions	Ref.
Pd-In/In ₂ O ₃ -250	99	95	1340	30 °C, 1 bar H ₂	[1]
PdZn/CN@ZnO	96	92	434	35 °C, 5 bar H ₂	[2]
Pd/ZnO/SMF	100	95	2556	35 °C, 5 bar H ₂	[3]
Pd(B,C)/OMC	100	95	3333	25 °C, 1 bar H ₂	[4]
UiO-67@Pd@UiO-67	100	92	15495	10 °C, 5 bar H ₂	[5]
Pd/NHPC-DETA-50	100	94	6846	90 °C, 3 bar H ₂	[6]
Pd ₃ S/C ₃ N ₄	85	100	300	30 °C, 1 bar H ₂	[7]
Pd@NMC-250(This Work)	97	91	5110	35 °C, 5 bar H ₂	

Notes and references

- [1] M. Tang, J. Deng, M. Li, X. Li, H. Li, Z. Chen and Y. Wang, *Green Chem.*, 2019, **21**, 4143.
- [2] L. Shen, S. Mao, J. Li, M. Li, P. Chen, H. Li, Z. Chen and Y. Wang, *J. Catal.*, 2017, **350**, 13.
- [3] N. Semagina, M. Grasmann, N. Xanthopoulos, A. Renken and L. Kiwi-Minsker, *J. Catal.*, 2007, **251**, 213.
- [4] Y. Yang, X. Zhu, L. Wang, J. Lang, G. Yao, T. Qin, Z. Ren, L. Chen, X. Liu, W. Li and Y. Wan, *Nature Commun.*, 2022, **13**, 2754.
- [5] K. Choe, F. Zheng, H. Wang, Y. Yuan, W. Zhao, G. Xue, X. Qiu, M. Ri, X. Shi, Y. Wang, G. Li and Z. Tang, *Angew. Chem. Int. Ed.*, 2020, **59**, 3650.
- [6] Q. Luo, Z. Wang, Y. Chen, S. Mao, K. Wu, K. Zhang, Q. Li, G. Lv, G. Huang, H. Li and Y. Wang, *ACS Appl. Mater. Interfaces*, 2021, **13**, 31775.
- [7] D. Albani, M. Shahrokhi, Z. Chen, S. Mitchell, R. Hauert, N. López and J. Pérez-Ramírez, *Nat. Commun.*, 2018, **9**, 2634.