Supporting information

π–π Electron Conjugation-Assisted Synthesis of a Robust Heterostructured CoO-MoO_2 Catalyst: Accelerated Ammonia Borane Hydrolysis for Hydrogen Evolution

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Calculation method for turnover frequency (TOF)

The calculation of the TOF value (min^{-1}) reference a typical method. The calculation equation used was as follows:

$$TOF = \frac{n(H_2)}{t \cdot n_{metal}} \quad (1)$$

wherein, $n(H_2)$ represents 2mmol hydrogen generated by hydrolysis of AB, t is the time corresponding to produce 2mmol hydrogen, and n_{metal} represents the total molar quantity of Co quantified by the ICP-OES measurement.

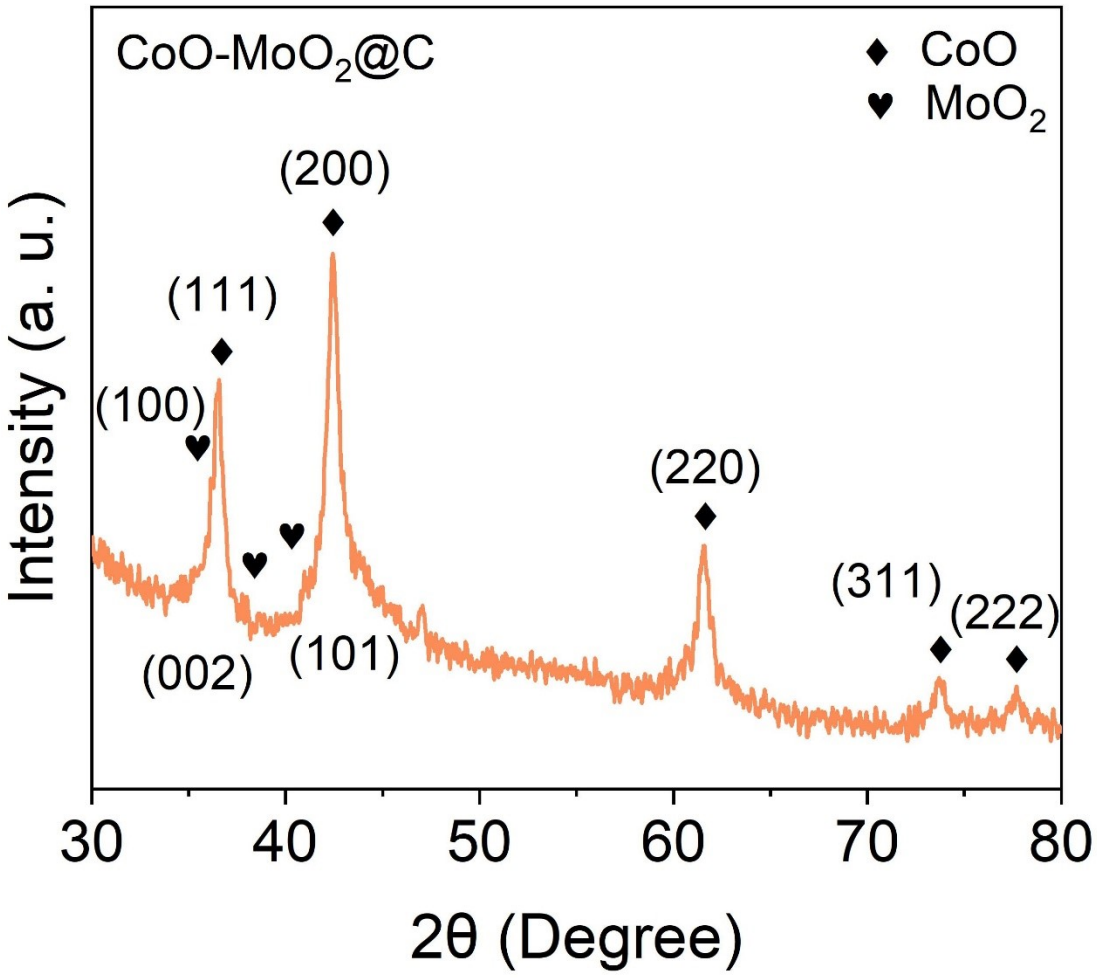

Figure S1. XRD pattern of CoO-MoO_2@C.

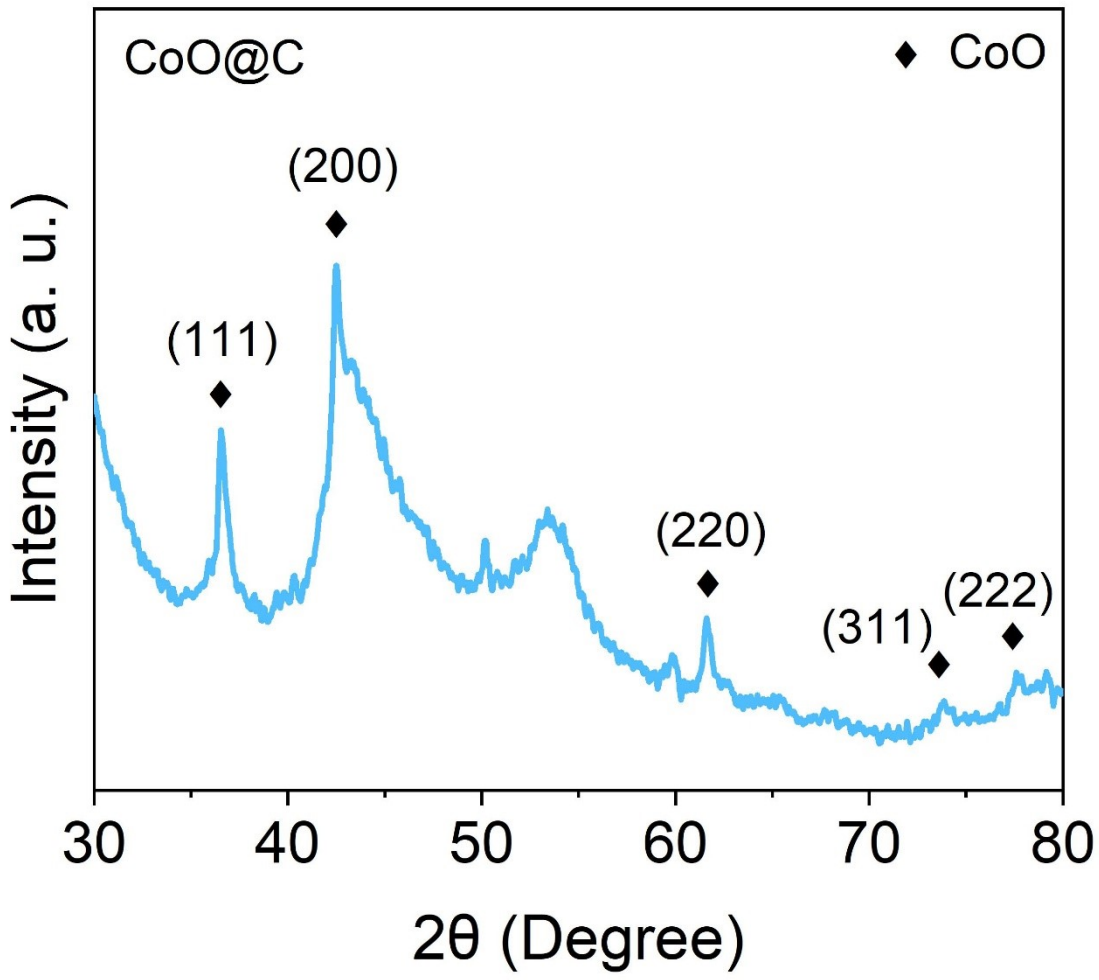

Figure S2. XRD pattern of CoO@C.

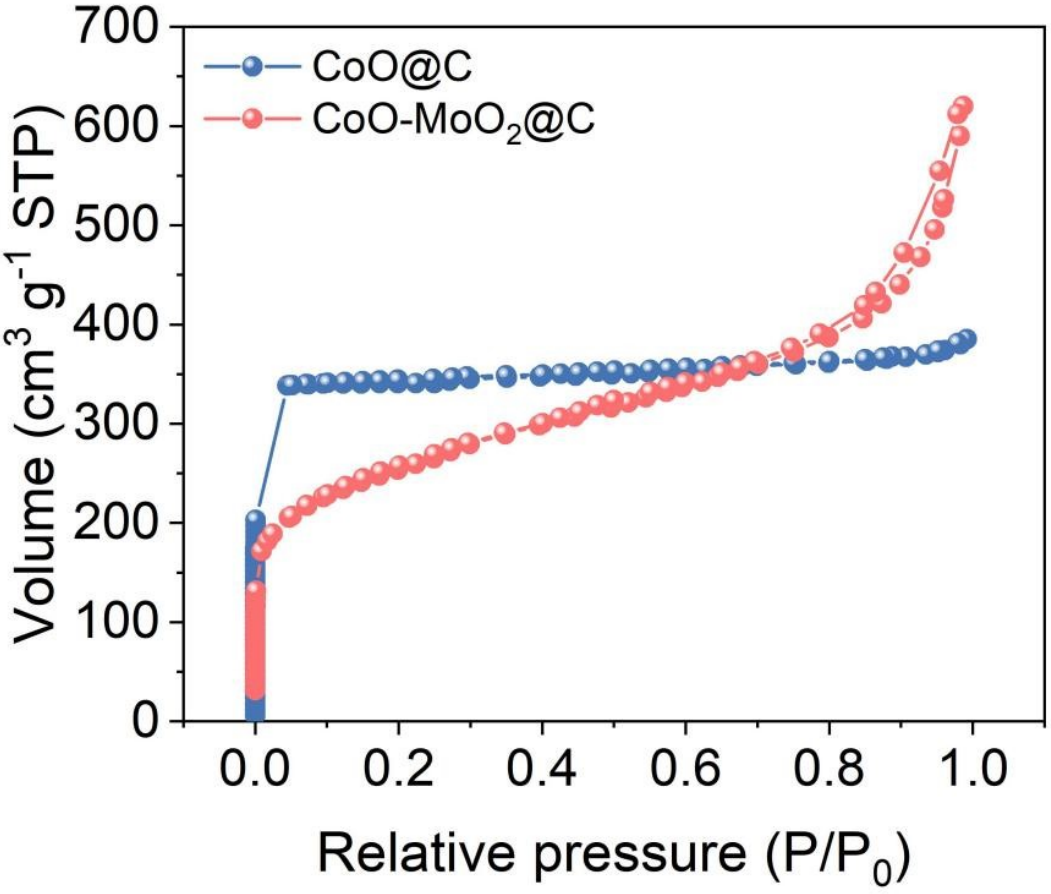

Figure S3. N_2 sorption isotherms of CoO@C and CoO-MoO_2@C.

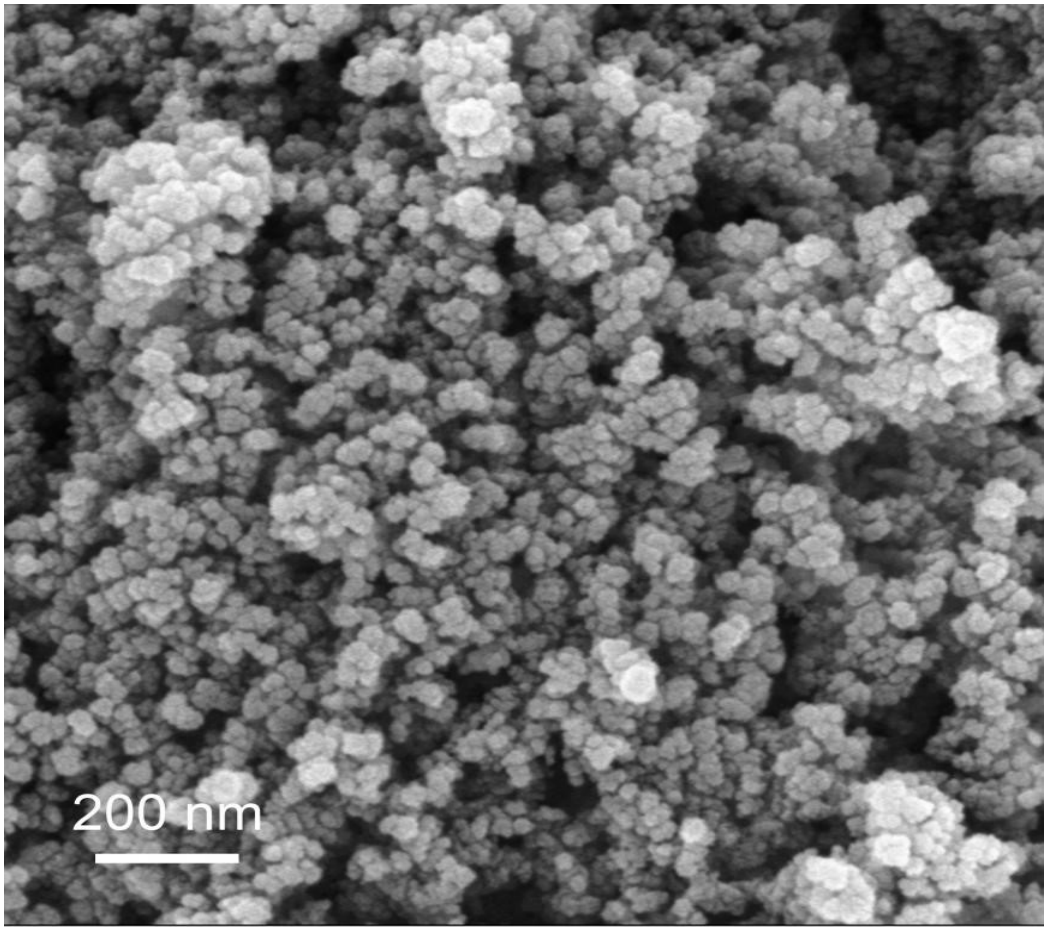

Figure S4. SEM image of CoO-MoO_2@C.

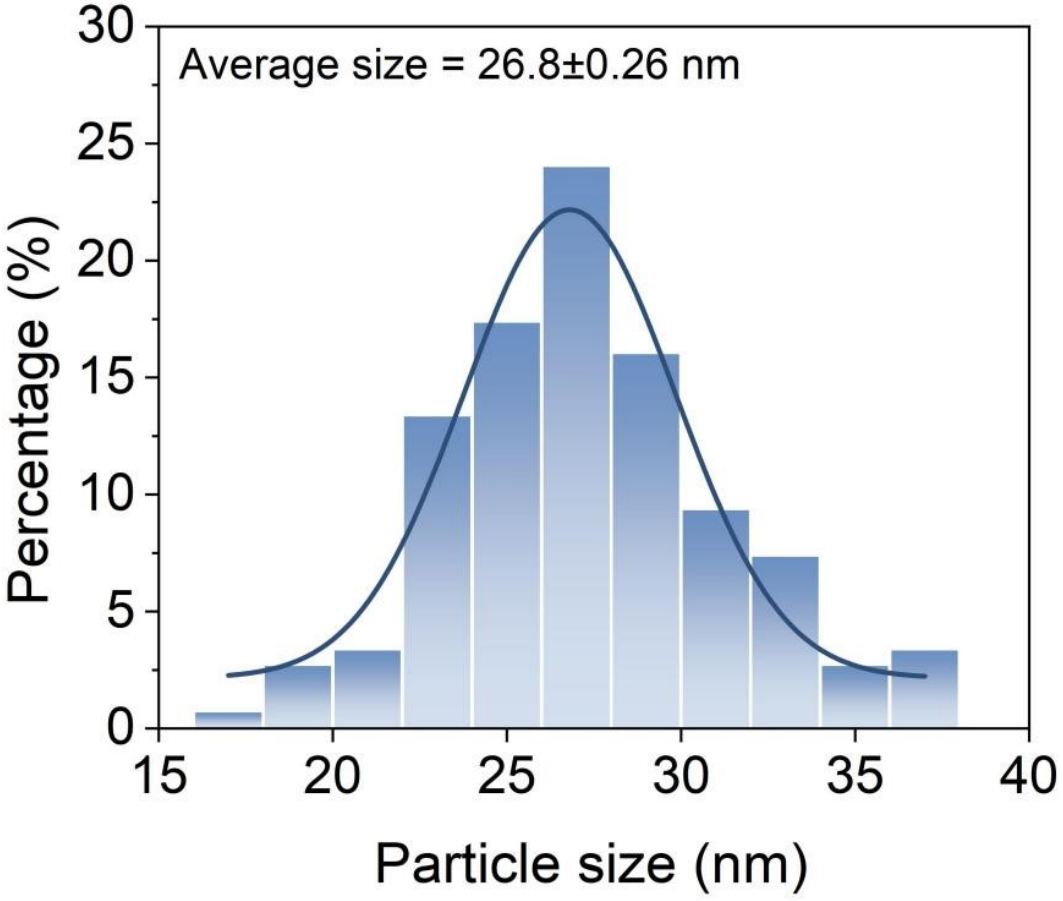

Figure S5. Particle size statistical result of CoO-MoO_2@C.

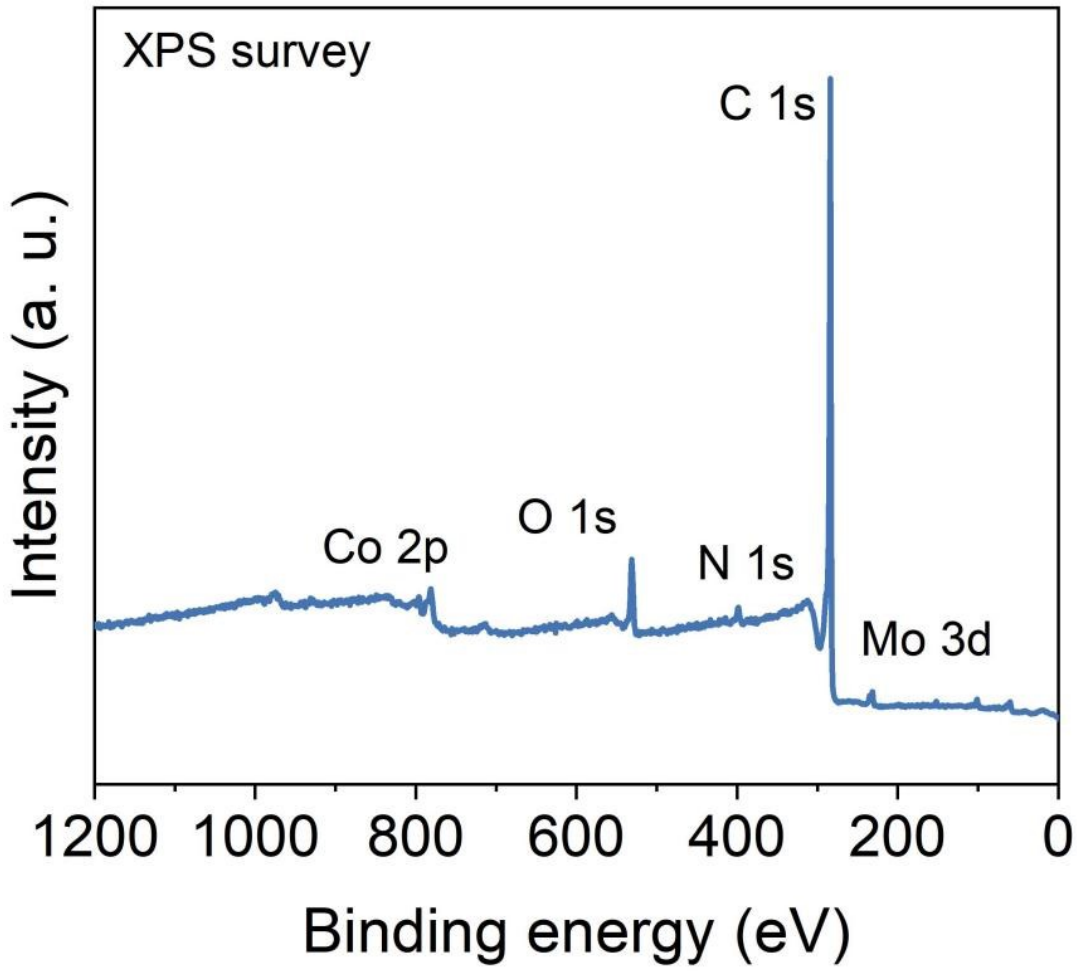

Figure S6. XPS spectra of CoO-MoO_2@C.

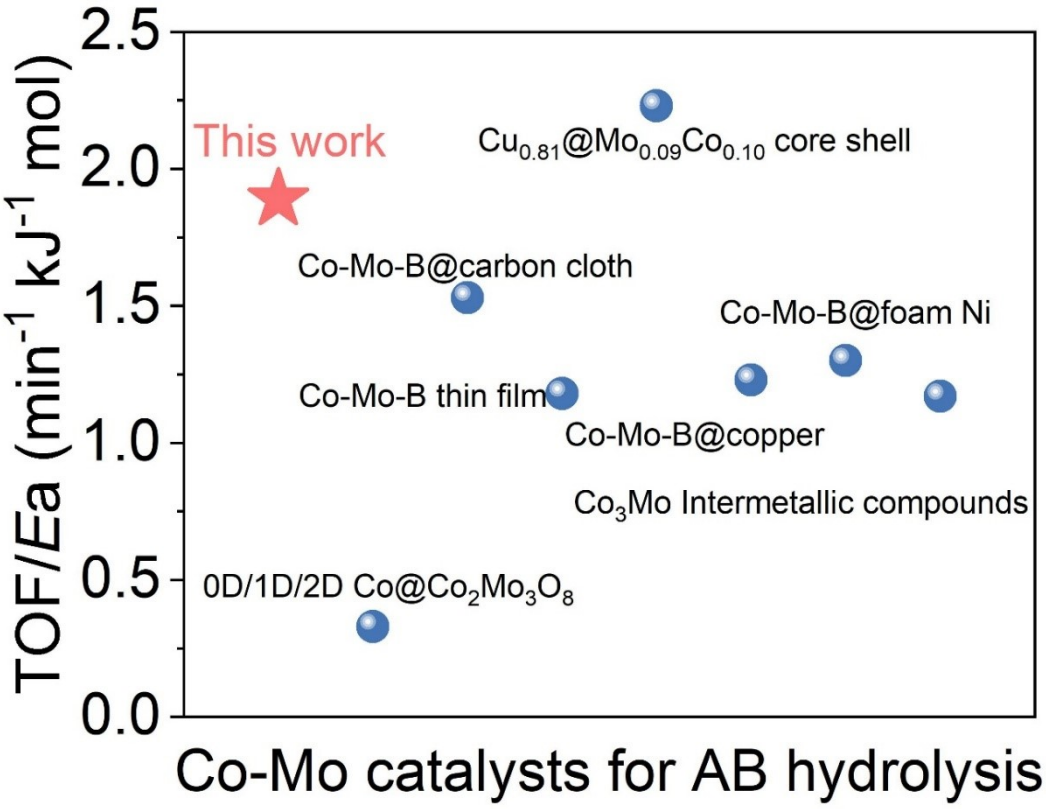

Figure S7. TOF/E_a of Co-Mo catalysts for AB hydrolysis.

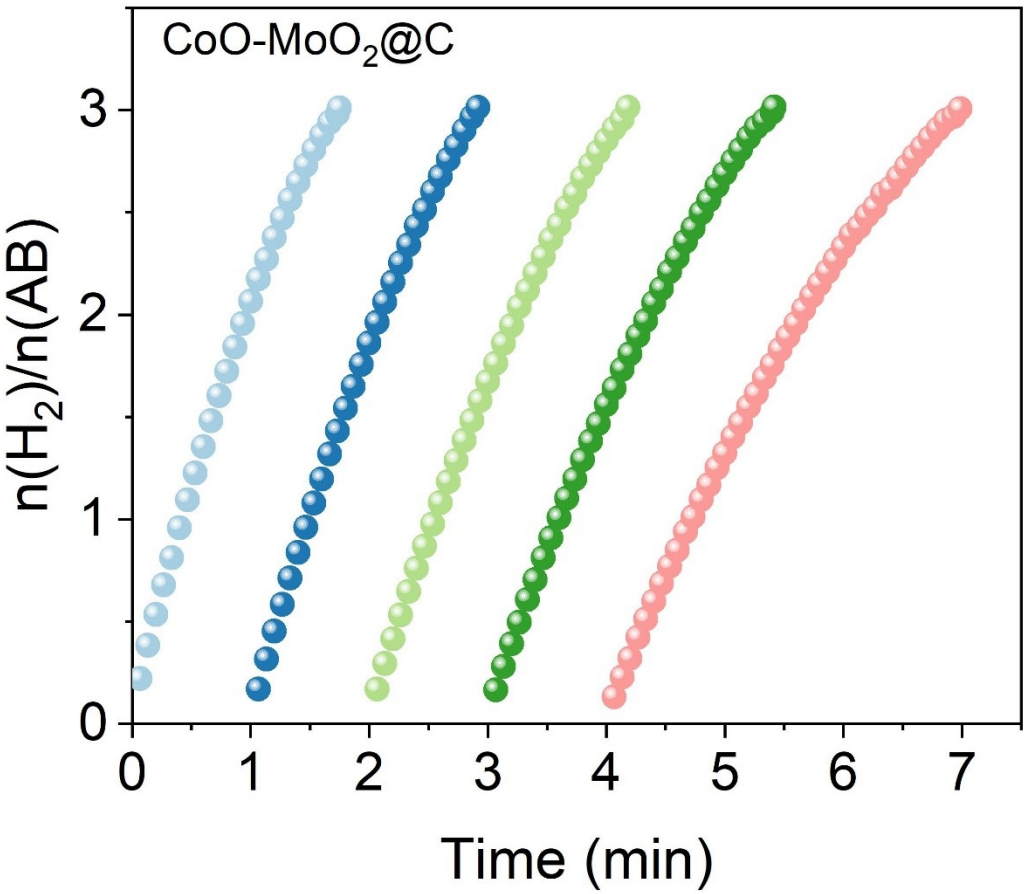

Figure S8. The cyclic stability test results of CoO-MoO_2@C.

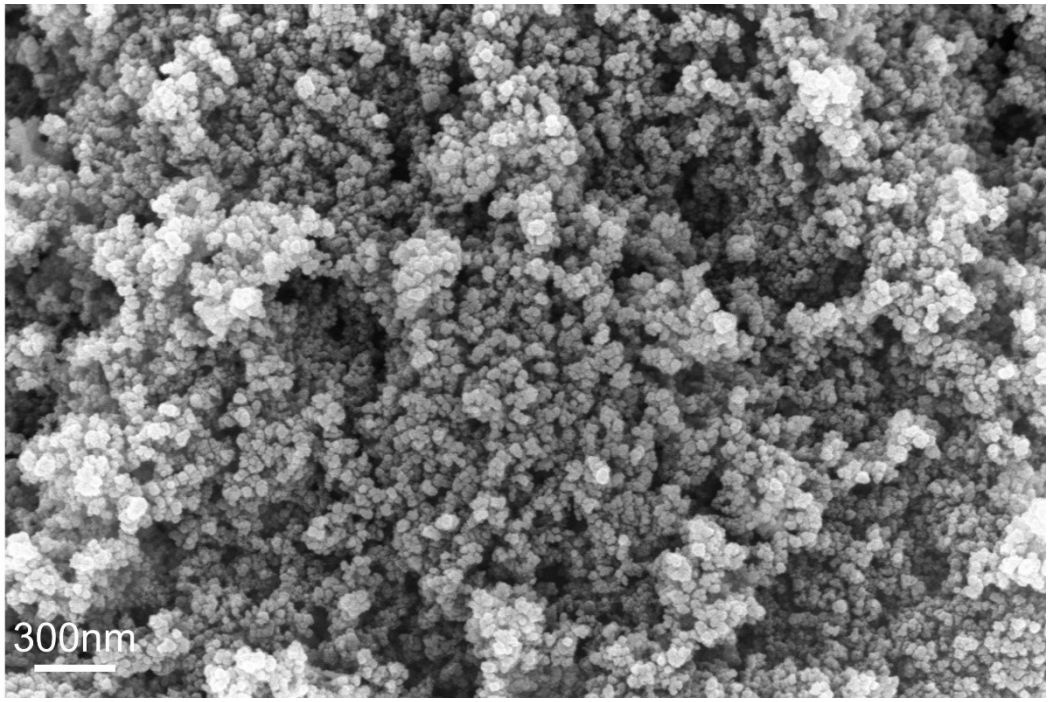

Figure S9. The SEM image of CoO-MoO_2@C after 5 cycles.

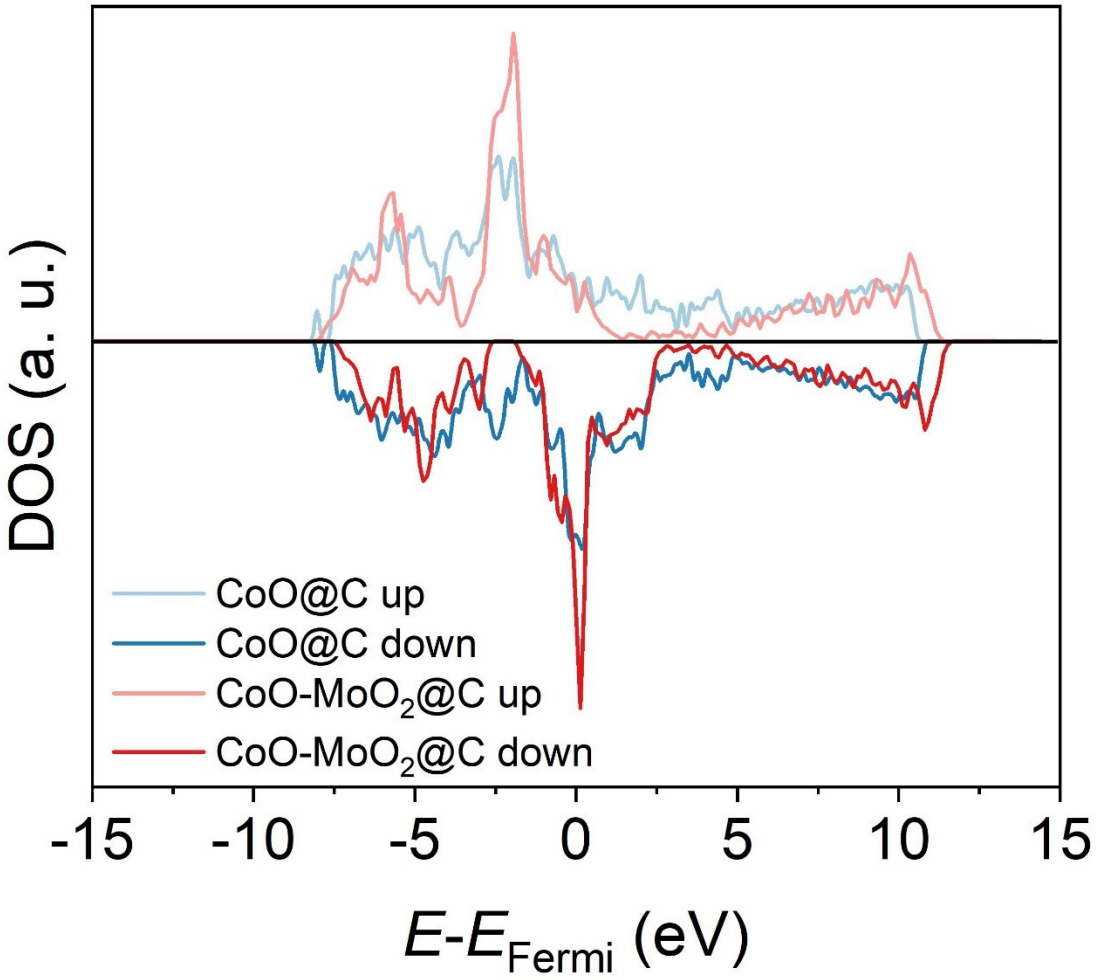

Figure S10. TDOS of CoO@C and CoO-MoO_2@C.

Tables

Table S1. Element contents from EDS mapping.

Elements	Atomic Fraction (%)	Mass Fraction (%)
C	88.44	78.32
N	1.31	1.36
O	8.18	9.66
Co	1.48	6.42
Mo	0.59	4.19

Table S2. Comparison of Co-based catalysts for the hydrolysis of AB at 298K.

Catalyst	NaOH (pH)	AB (mg)	TOF (mol_{H2}·mol^{-1}·min^{-1})	E_a (kJ mol^{-1})	TOF/E_a （min^{-1}·kJ^{-1}·mol）	Ref.
CoO-MoO_2 @C	14	30	55.4	29.3	1.89	This work
0D/1D/2D Co@$Co_2Mo_3O_8$	14.3	20	17.3	51.8	0.33	1
Co-Mo-B@carbon cloth	11.5	40	38.6	25.2	1.53	2
Co-Mo-B thin film	11	40	49.3	41.7	1.18	3
$Cu_{0.81}$@$Mo_{0.09}$ $Co_{0.10}$ core shell	---	60	49.6	22.2	2.23	4
Co-Mo-B @ copper	11	40	72.7	59.3	1.23	5
Co-Mo-B@foam Ni	11.5	40	59.2	45.5	1.30	6
Co_3Mo Intermetallic compounds	14.2	20	40.2	34.43	1.17	7

Reference

1. J. He, Z. Huang, W. Chen, X. Xiao, Z. Yao, Z. Liang, L. Zhan, L. Lv, J. Qi, X. Fan and L. Chen, *Chemical Engineering Journal*, 2022, **431**.
2. Y. Wang, K. Zou, D. Zhang, G. Li, W. Meng, D. Wang, Z. Cao, K. Zhang and S. Wu, *International Journal of Hydrogen Energy*, 2020, **45**, 14418-14427.
3. C. Li, W. Meng, G. Hu, Y. Wang, Z. Cao and K. Zhang, *International Journal of Hydrogen Energy*, 2018, **43**, 17664-17672.
4. C. Wang, H. Wang, Z. Wang, X. Li, Y. Chi, M. Wang, D. Gao and Z. Zhao, *International Journal of Hydrogen Energy*, 2018, **43**, 7347-7355.
5. Y. Wang, W. Meng, D. Wang, Z. Wang, K. Zou, Z. Cao, K. Zhang, S. Wu and G. Li, *International Journal of Hydrogen Energy*, 2019, **44**, 23267-23276.
6. Y. Wang, D. Wang, C. Zhao, W. Meng, T. Zhao, Z. Cao, K. Zhang, S. Bai and G. Li, *International Journal of Hydrogen Energy*, 2019, **44**, 10508-10518.
7. J. He, P. Zhou, X. Xiao, F. Chu, L. Ouyang, B. Liu, R. Li, Z. Huang, L. Hu, S. Yuan, T. Zhou, X. Fan and L. Chen, *Chemical Engineering Journal*, 2023, **474**.