Supporting Information

Cobalt-Molybdenum synergistic catalysis for hydrogenolysis of terephthalate-based polyesters

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1. General Information

All chemical reagents are obtained from commercial suppliers and used without further purification. ^{1}H NMR spectra are recorded on an AVANCE III Bruker spectrometer operating at 500 MHz. Some products were analyzed by gas chromatography-mass spectroscopy (GC-MS) with a Thermo Scientific Trace 1300 GC/MS instrument equipped with TR-5MS columns.

2. ICP-MS results of prepared catalysts

Table S1. ICP-MS analysis of prepared catalysts

Catalyst	Element	Metal Content (mg/kg)	Molar Ratio (Co/Mo)
CoMo@NC	Co	43023.5	3.45
	Mo	20265.4	
	Zn	209.4	
Co@NC	Co	45578.1	-
	Zn	144.8	
Mo@NC	Mo	25944.8	-
	Zn	276.9	
CoMo@NC[a]	Co	42691.8	3.30
	Mo	20657.3	
	Zn	218.6	

[a] CoMo@NC after 6 runs.

3. SEM images

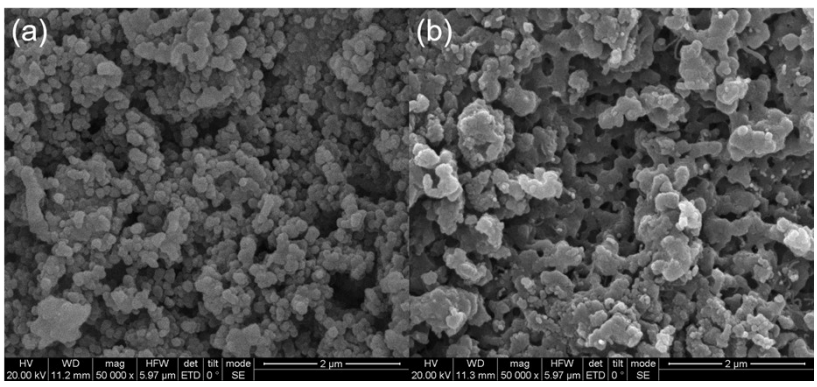

Fig. S1 SEM images of (a) Mo@ZIF-CoZn, (b) CoMo@NC.

4. NH_3-TPD profiles

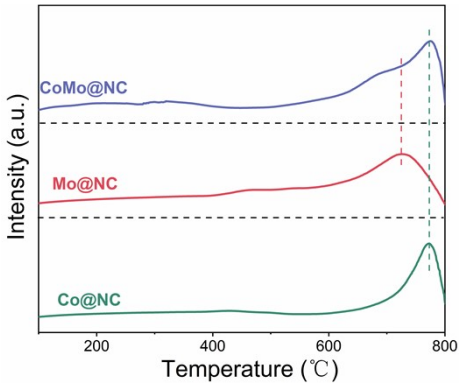

Fig. S2 NH_3-TPD profiles of CoMo@NC, Mo@NC and Co@NC.

5. XPS survey spectra

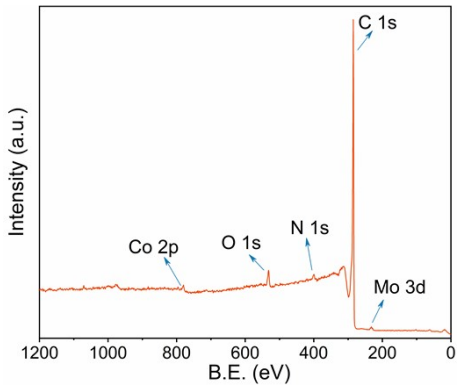

Fig. S3 XPS survey spectra of CoMo@NC.

6. Raman spectra

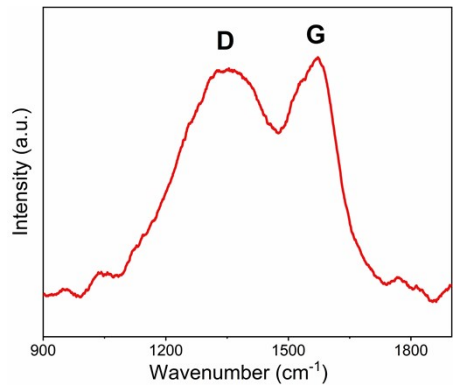

Fig. S4 Raman spectra of CoMo@NC.

7. Porous nature of CoMo@NC

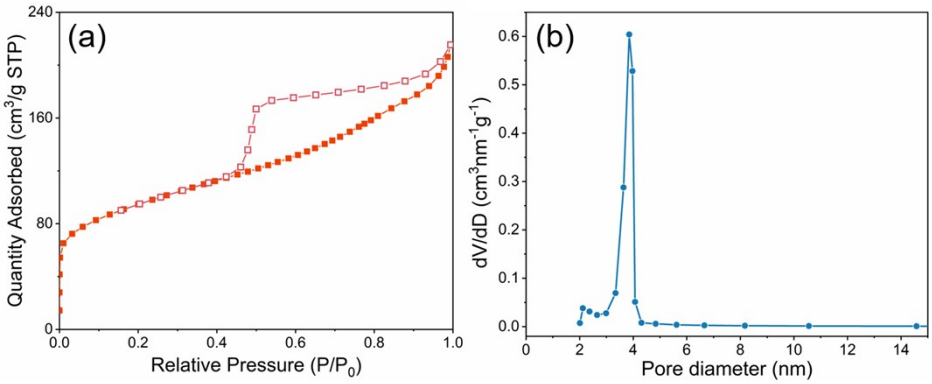

Fig. S5 (a) N_2 adsorption/desorption isotherms of CoMo@NC, (b) the corresponding pore size distributions.

8. Rection tube and samples

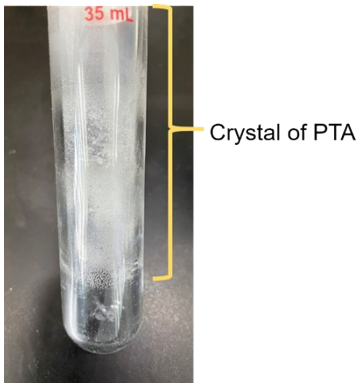

Fig. S6 Reaction tube after the hydrogenolysis of PET.

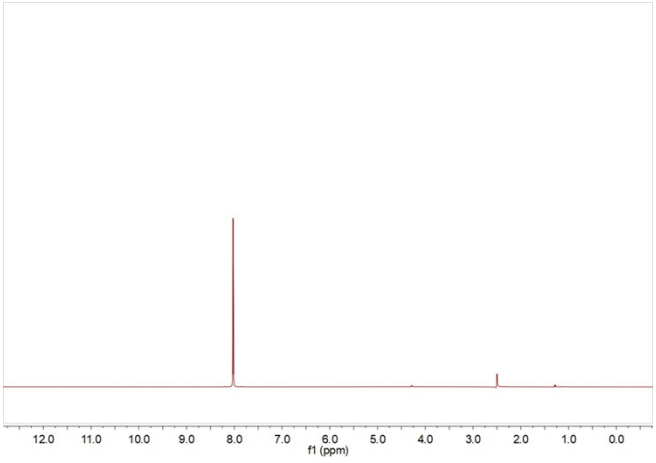

Fig. S7 ^{1}H NMR spectrum of reaction product with d_6-DMSO as the solvent.

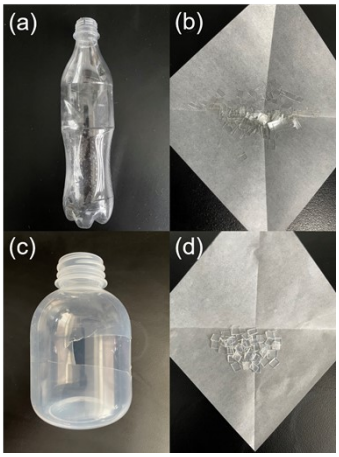

Fig. S8 (a) PET bottle, (b) PET pieces, (c) PP bottle, (d) PP pieces.

9. GC spectra

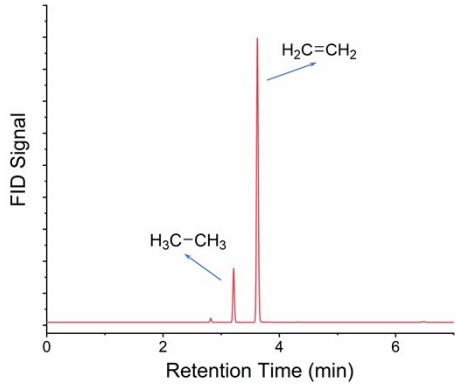

Fig. S9 GC spectra of the gas phase product of the reaction (Table 1, entry 2).

10. Time-course monitoring

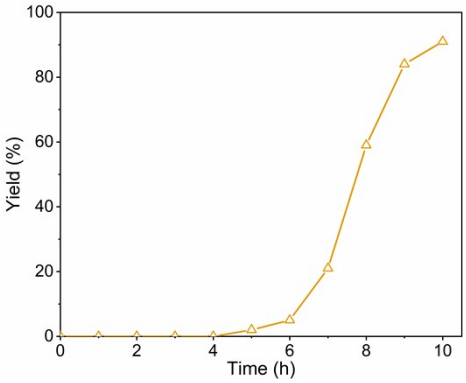

Fig. S10 Time-course monitoring of the reaction. Reaction conditions: 100 mg PET, 1 atm H2 (balloon), 260 °C, 30 mg CoMo@NC. Isolated yields of PTA. After isolating sublimated PTA, DMSO was added to dissolute and detect any other product remained in the tube.

11. Deuterium labeling experiment

The model molecule deuterated d_4-1,2-ethanediol dibenzoate (**4-d_4**) was synthesized according to a reported procedure for 1,2-ethanediol dibenzoate [1], in the procedure, d_6-ethylene glycol was used instead of ethylene glycol.

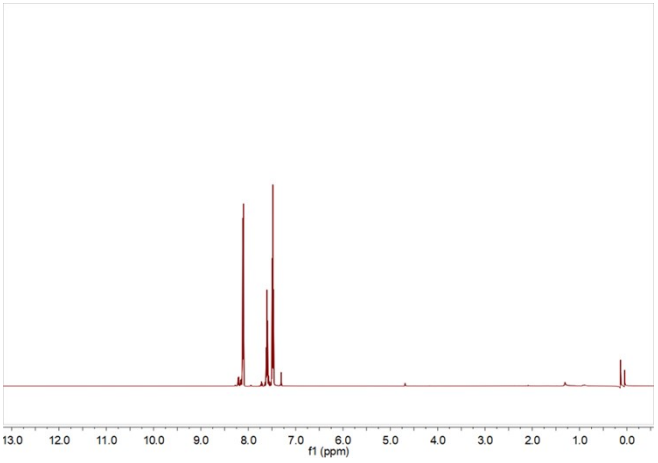

Fig. S11 ^{1}H NMR spectrum of **4-d_4**, $CDCl_3$ was used as the solvent.

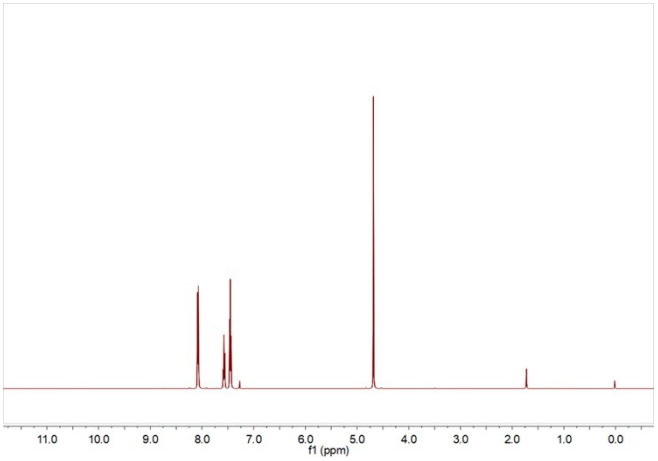

Fig. S12 ^{1}H NMR spectrum of 1,2-ethanediol dibenzoate sample, $CDCl_3$ was used as the solvent.

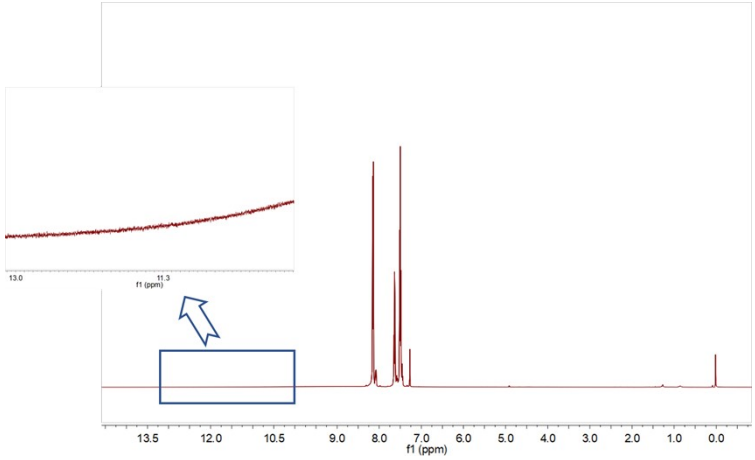

Fig. S13 ^{1}H NMR spectrum of product of scheme 2a, $CDCl_3$ was used as the solvent.

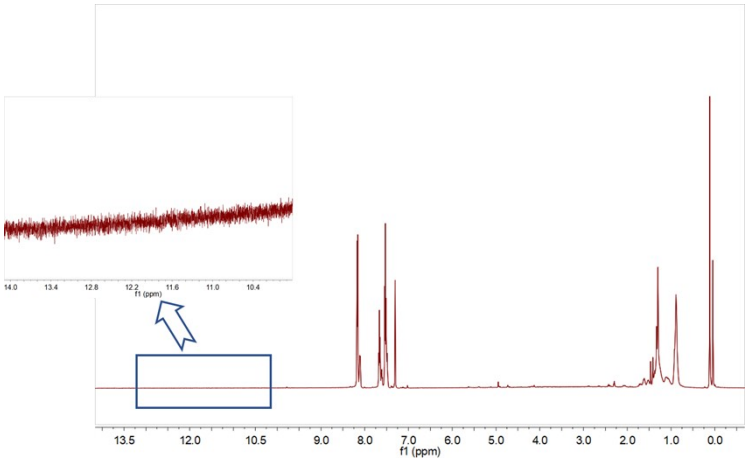

Fig. S14 ^{1}H NMR spectrum of product of scheme 2b, $CDCl_3$ was used as the solvent.

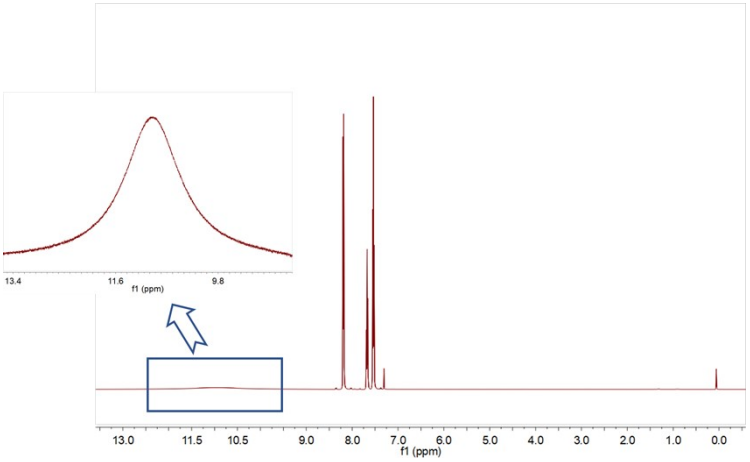

Fig. S15 ^{1}H NMR spectrum of benzoic acid sample, $CDCl_3$ was used as the solvent.

12. Characterization of the recycled catalyst

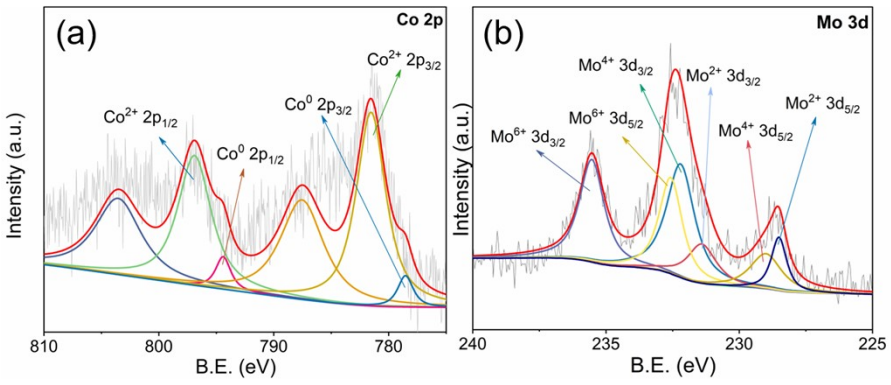

Fig. S16 XPS spectra of the (a) Co 2p region, (b) Mo 3d region of recycled CoMo@NC.

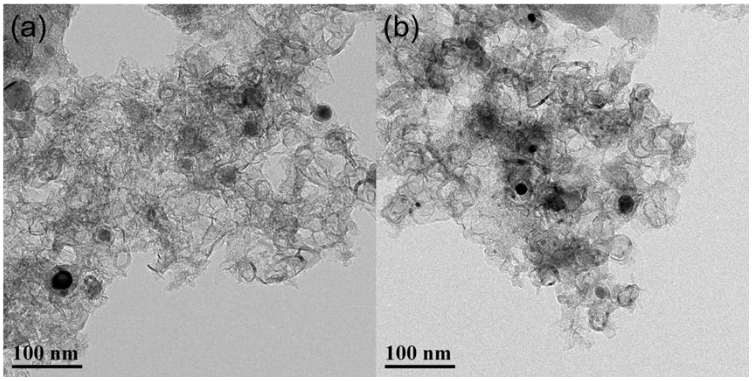

Fig. S17 TEM image of CoMo@NC after (a) first cycle, (b) sixth cycle.

Reference

[1] M.K. Grachev, A.A. Charaev, G.I. Kurochkina, T.A. Batalova, N.O. Soboleva, L.K. Vasyanina, E.E. Nifant'ev, Russ. J. Gen. Chem. 81 (2011) 2129-2135. https://doi.org/10.1134/S1070363211100161.