

Supporting Information

Hydroxylation of benzene to phenol over heteropoly acid $\text{H}_5\text{PMo}_{10}\text{V}_2\text{O}_{40}$ supported onto amine-functionalized MCM-41

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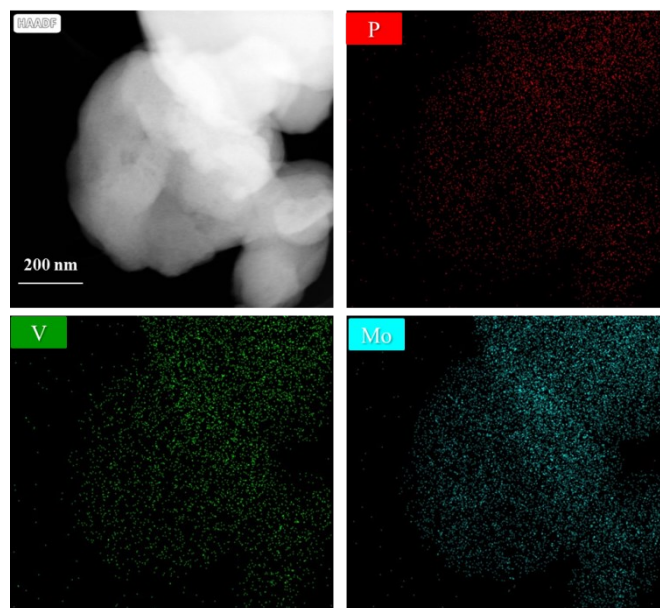


Fig. S1. The results of element mapping for HPMoV/MCM-41.

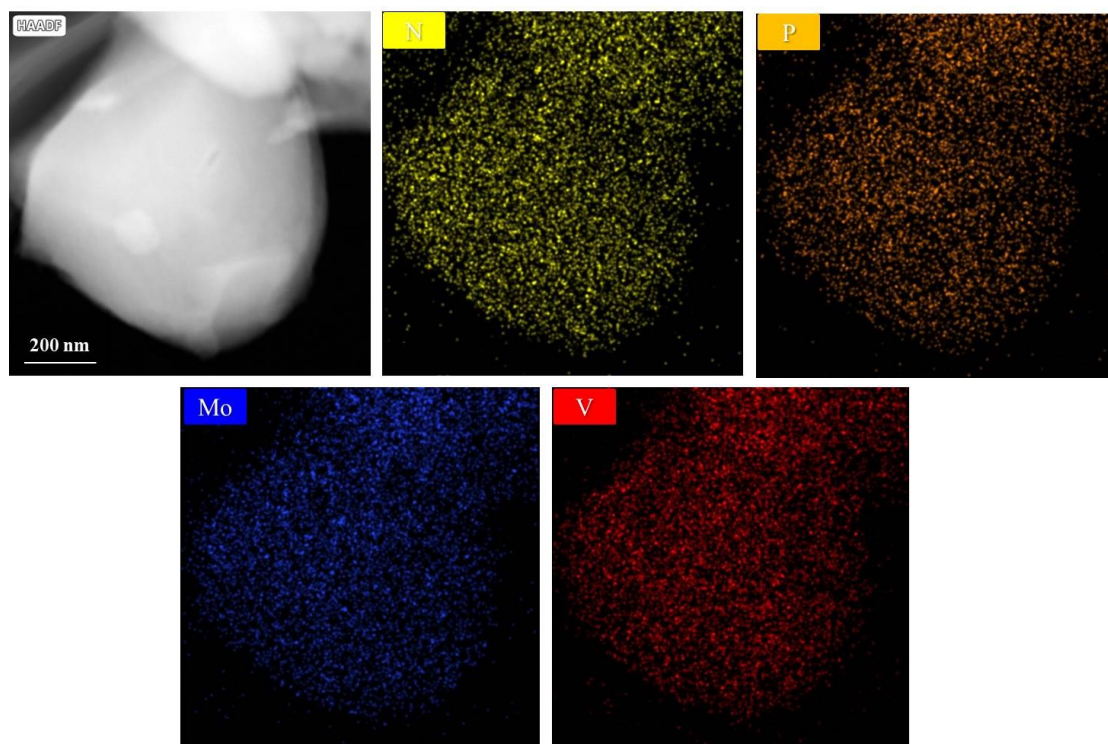


Fig. S2. The results of element mapping for HPMoV[ethanol]/MCM-41-NH₂.

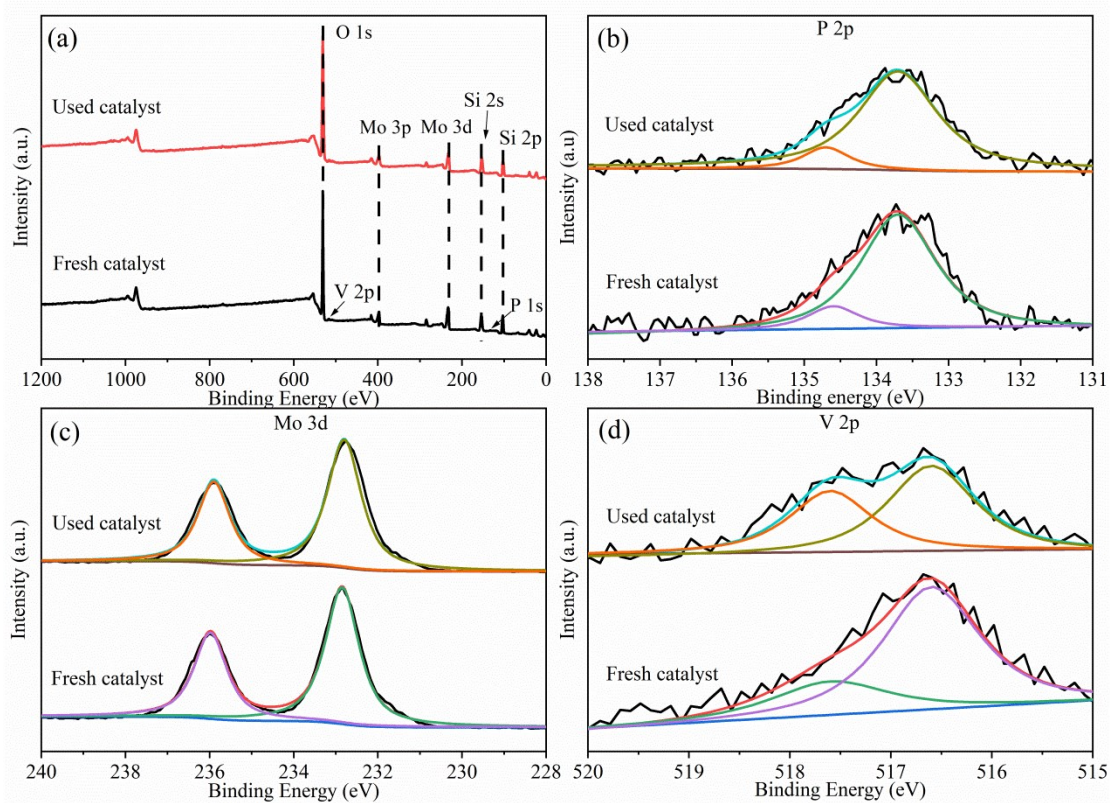


Fig. S3. XPS spectra of (a) survey spectra, (b) P 2p, (c) Mo 3d, (d) V 2p, for the fresh and used

HPMoV/MCM-41

Carbon Balance

Table S1 Calculation of carbon balance (CB) for the oxidation of benzene over prepared catalysts.

Entry	Catalysts	C before oxidation (mmol)		C after oxidation (mmol)				CB(%)
		BZ	BZ	PH	HQ	BQ	Total	
1	MCM-41	203.1	201.9	0.5±0.03	-	-	202.4	99.6
2	MCM-41-NH ₂	203.1	201.9	0.6±0.03	-	-	202.5	99.7
3	HPMoV	203.1	156.7±0.3	44.4±0.3	0.8±0.04	0.5±0.04	202.4	99.6
4	HPMoV	203.1	159.6±0.3	40.9±0.3	0.7±0.03	0.5±0.03	201.7	99.3
5	HPMoV/MCM-41	203.1	167.6±0.4	33.7±0.3	0.7±0.03	0.5±0.03	202.5	99.7
6	HPMoV[ethanol]/MCM-41-NH ₂	203.1	159.4±0.3	41.5±0.4	0.8±0.02	0.4±0.04	202.1	99.5
7	HPMoV[water]/MCM-41-NH ₂	203.1	162.1±0.3	38.3±0.4	1.1±0.03	0.4±0.05	201.9	99.4

Reaction conditions: benzene (3.0 mL, 33.4 mmol), H₂O₂/benzene=3:1, catalyst (200 mg), mixed solvent of acetonitrile and acetic acid (30 mL, volume ratio 1:1), 70 °C, 9 h

BZ: benzene; PH: phenol; HQ: hydroquinone; BQ: benzoquinone; CB: carbon balance;

Carbon balance (CB) = [$\frac{\text{(total no. of carbon (in mmol) present in the reaction mixture after catalysis)}}{\text{(total no. of carbon (in mmol) present in the reaction mixture before catalysis)}} \times 100$] %.