Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Influence and stability of the surface density of MoO_x on TiO_2 in deoxydehydration: Structure-activity correlations

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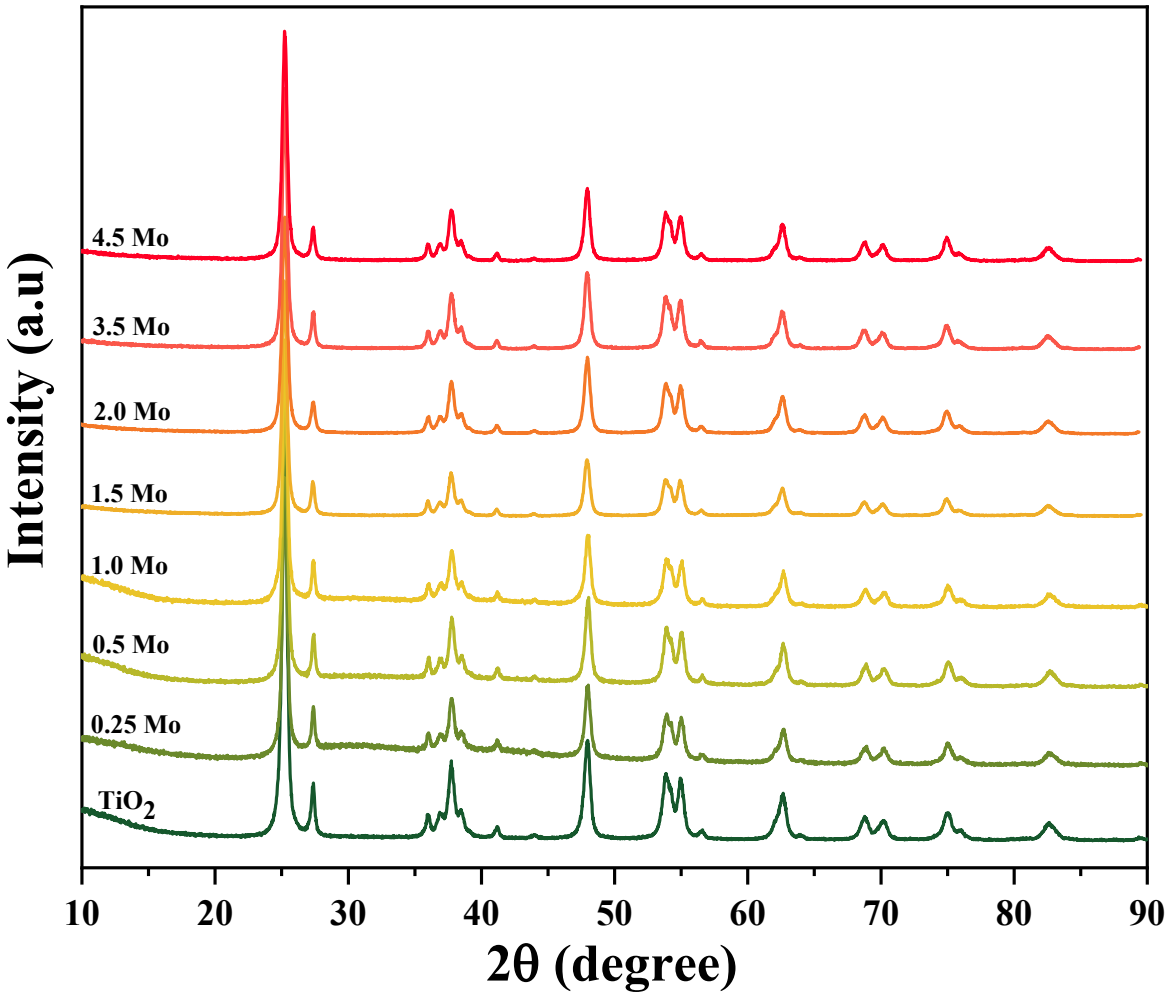


Fig. S1 XRD patterns of catalysts containing different surface densities of MoO_x.

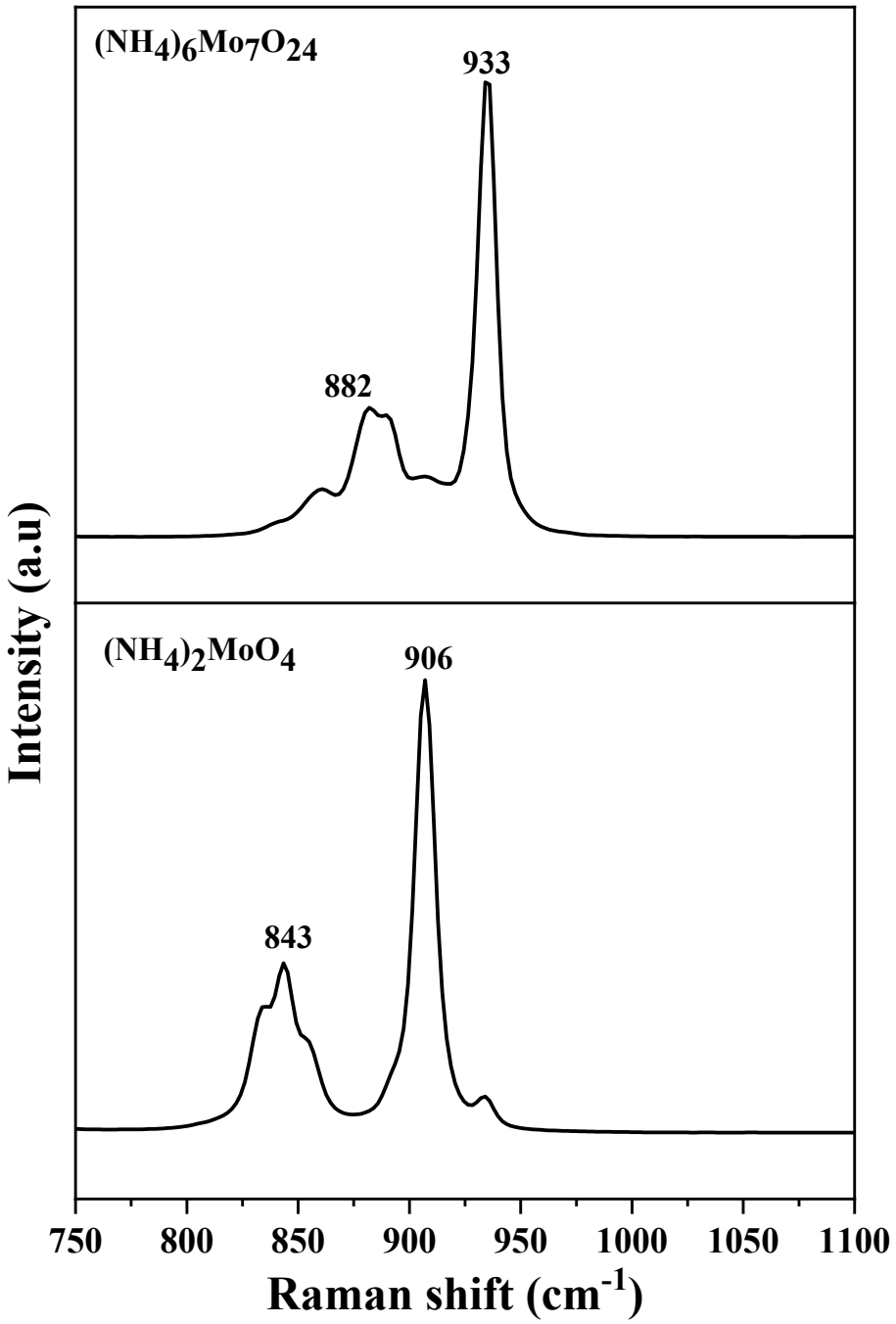


Fig. S2 Raman spectra of monomeric precursor $(NH_4)_2MoO_4$ and polymeric $(NH_4)_6Mo_7O_{24}$ showing precursor Mo=O stretching peaks at 906 and 933 cm^{-1} respectively.

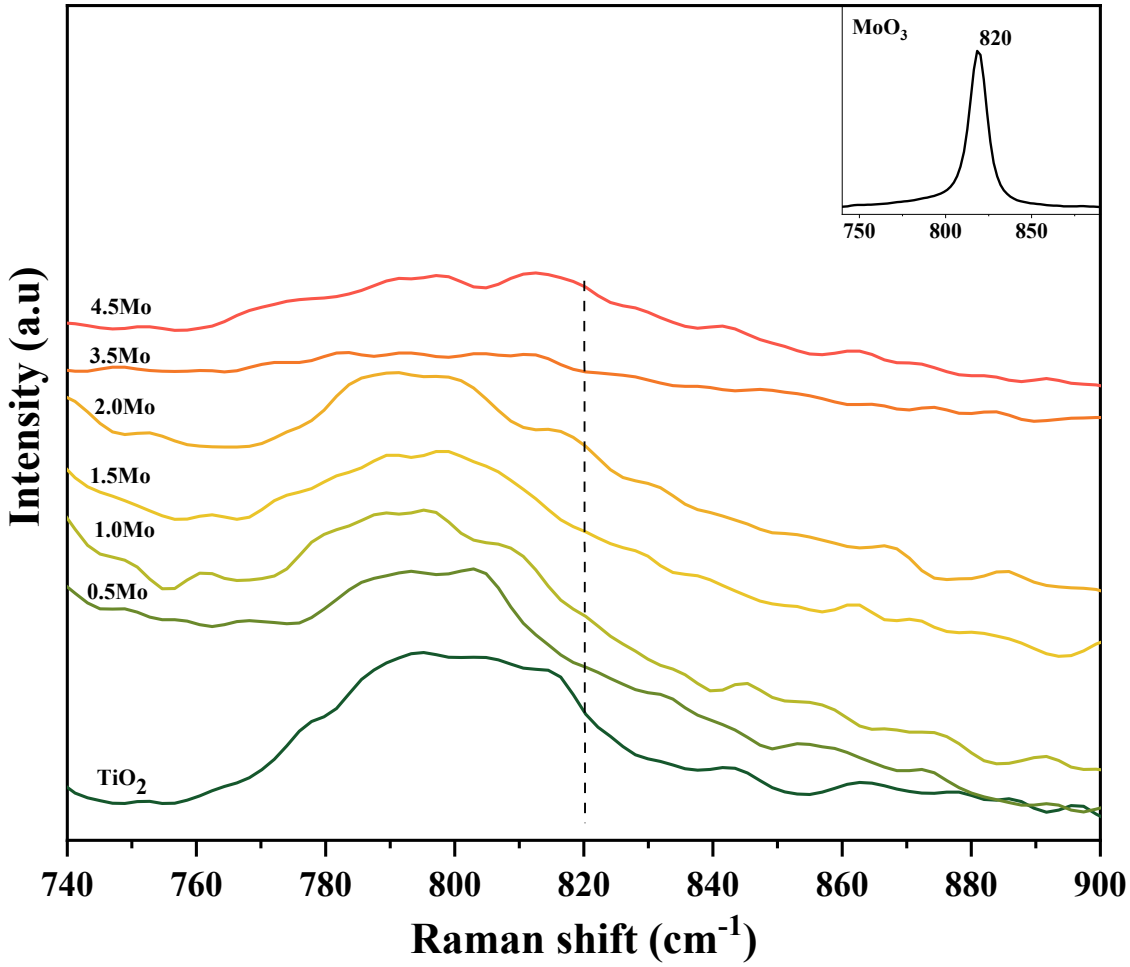


Fig. S3 Raman spectra of the catalysts in the 820 cm^{-1} range.

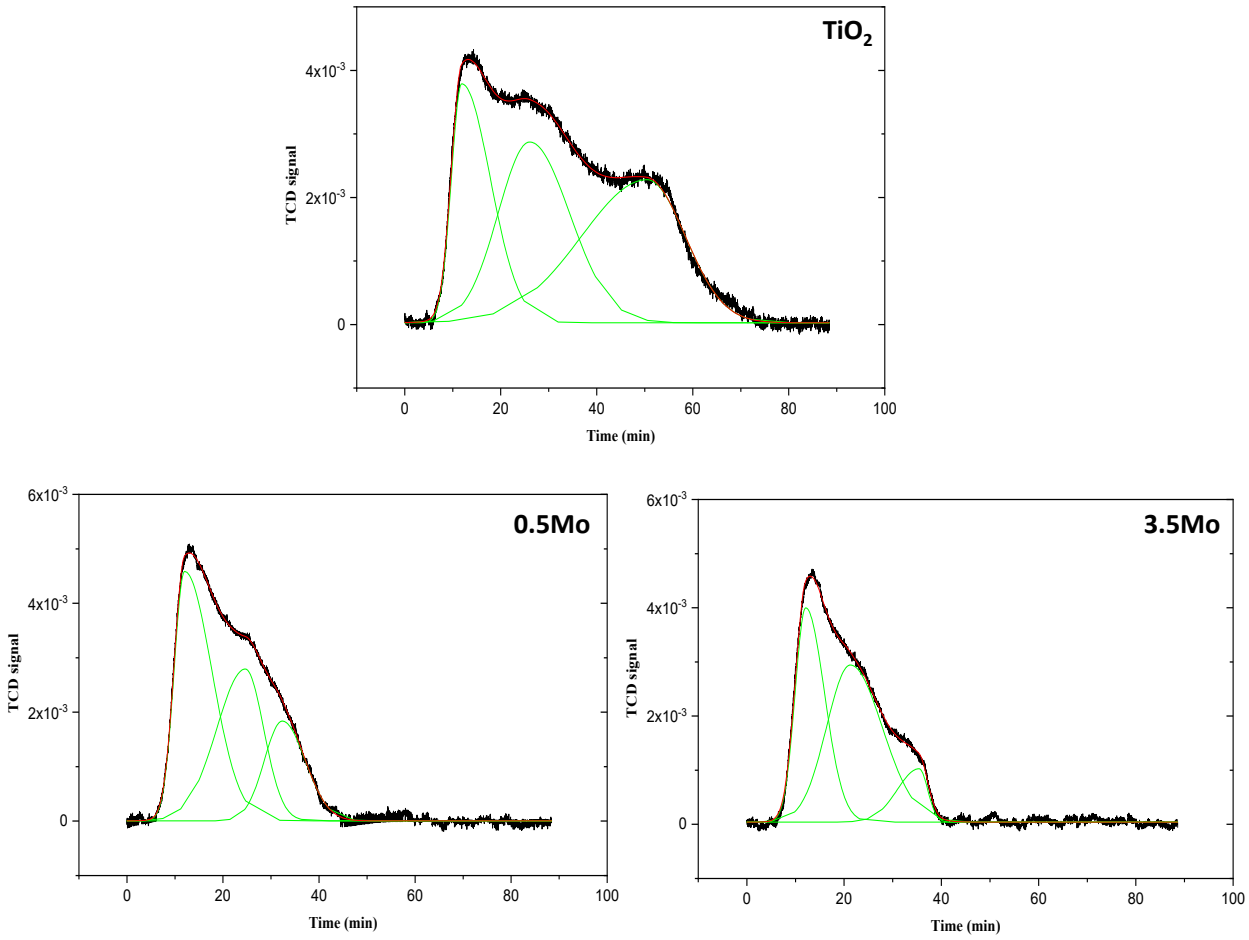


Fig. S4 NH_3-TPD deconvolution graphs of TiO_2, 0.5Mo, and 3.5Mo catalysts.

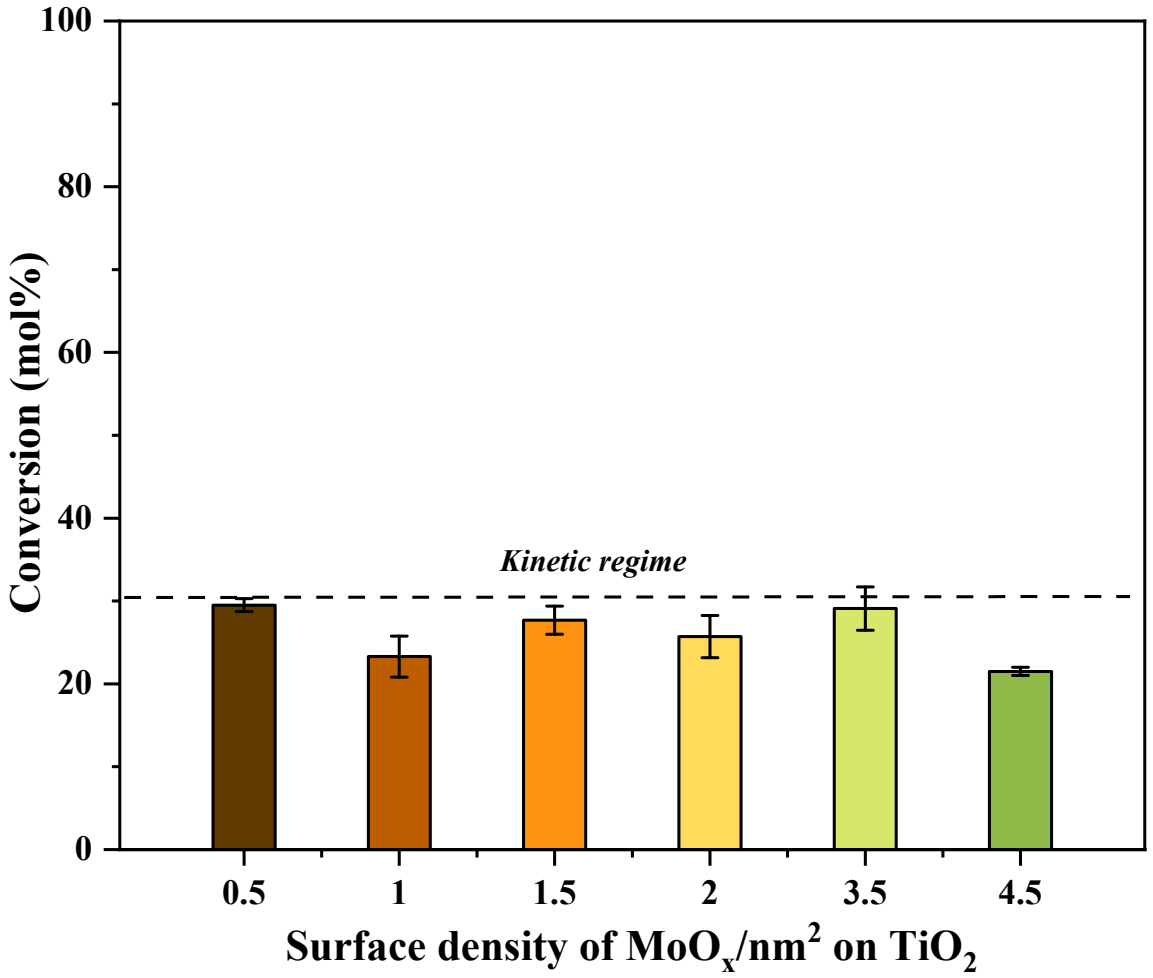


Fig S5. Conversion and yield of MoO_x/TiO_2 in the kinetic regime with different surface densities of Mo. *Reaction conditions:* 1,4-AHE = 0.6 mmol, 3-Octanol = 6 mmol, Mo = 0.4-0.8 mol% w.r.t 1,4-AHE, T = 200°C, t = 18 h.

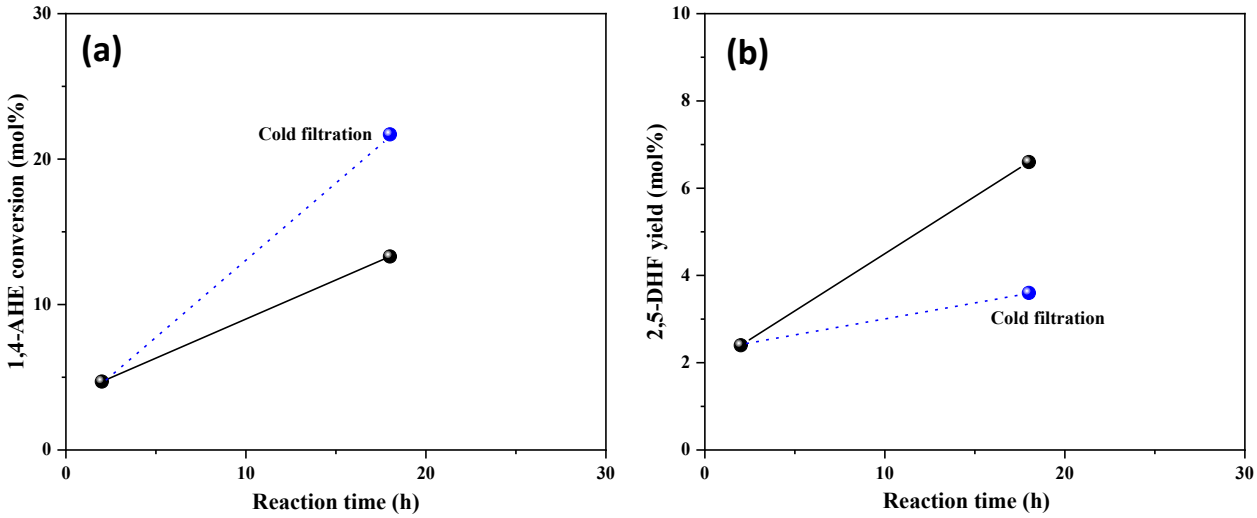


Fig. S6 Leaching studies of dried 0.5Mo catalyst. (a) Reaction time *versus* 1,4-AHE conversion, and (b) reaction time *versus* 2,5-DHF yield. *Reaction conditions:* 1,4-AHE = 0.6 mmol, 3-Octanol = 6 mmol, Mo = 0.4 mol% w.r.t 1,4-AHE, T = 200^{o}C.

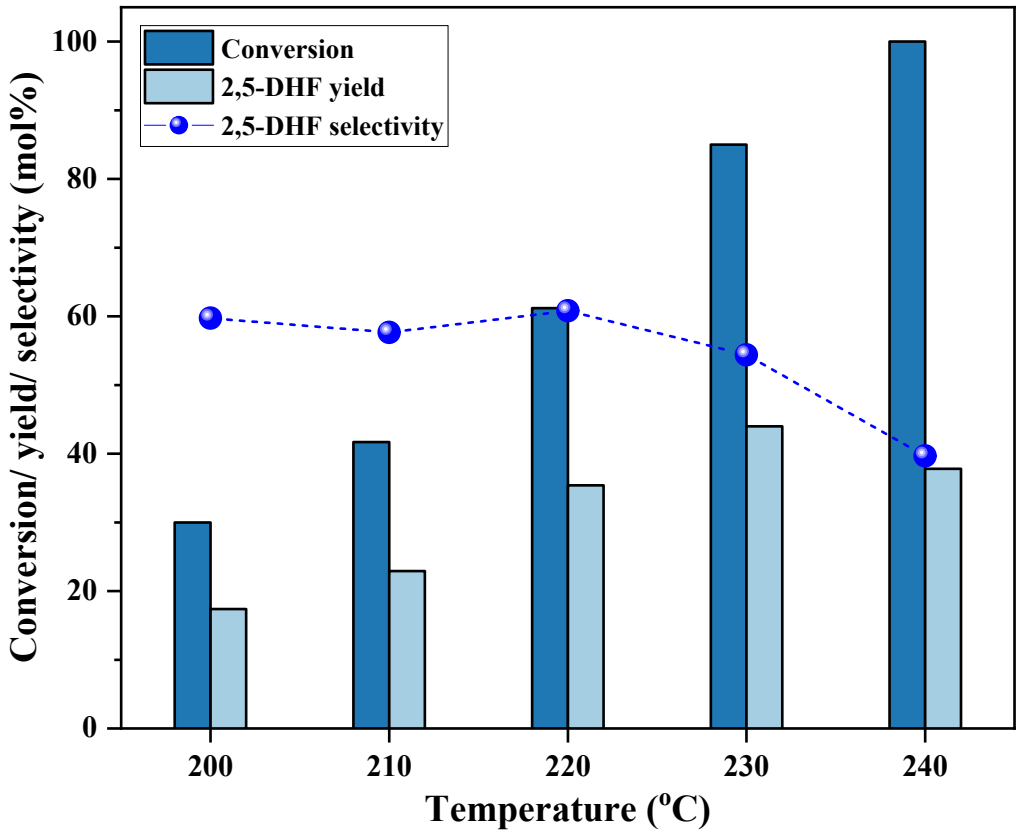


Fig. S7 Effect of temperature on 1,4-AHE conversion, 2,5-DHF yield, 2,5-DHF selectivity of 0.5Mo catalyst. *Reaction conditions:* 1,4-AHE = 0.6 mmol, 3-Octanol = 6 mmol, Mo = 0.4 mol% w.r.t 1,4-AHE, t = 18 h.

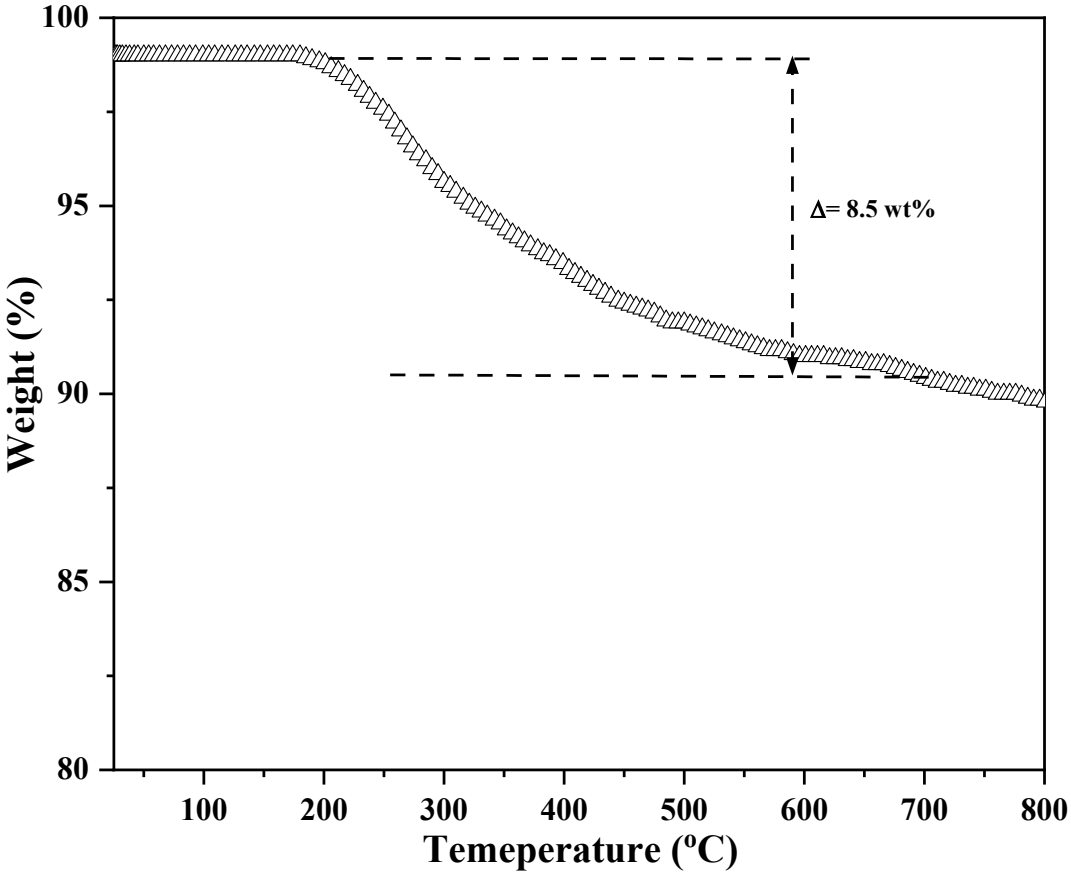


Fig S8. TGA analysis of the catalyst after its third recycle experiment.

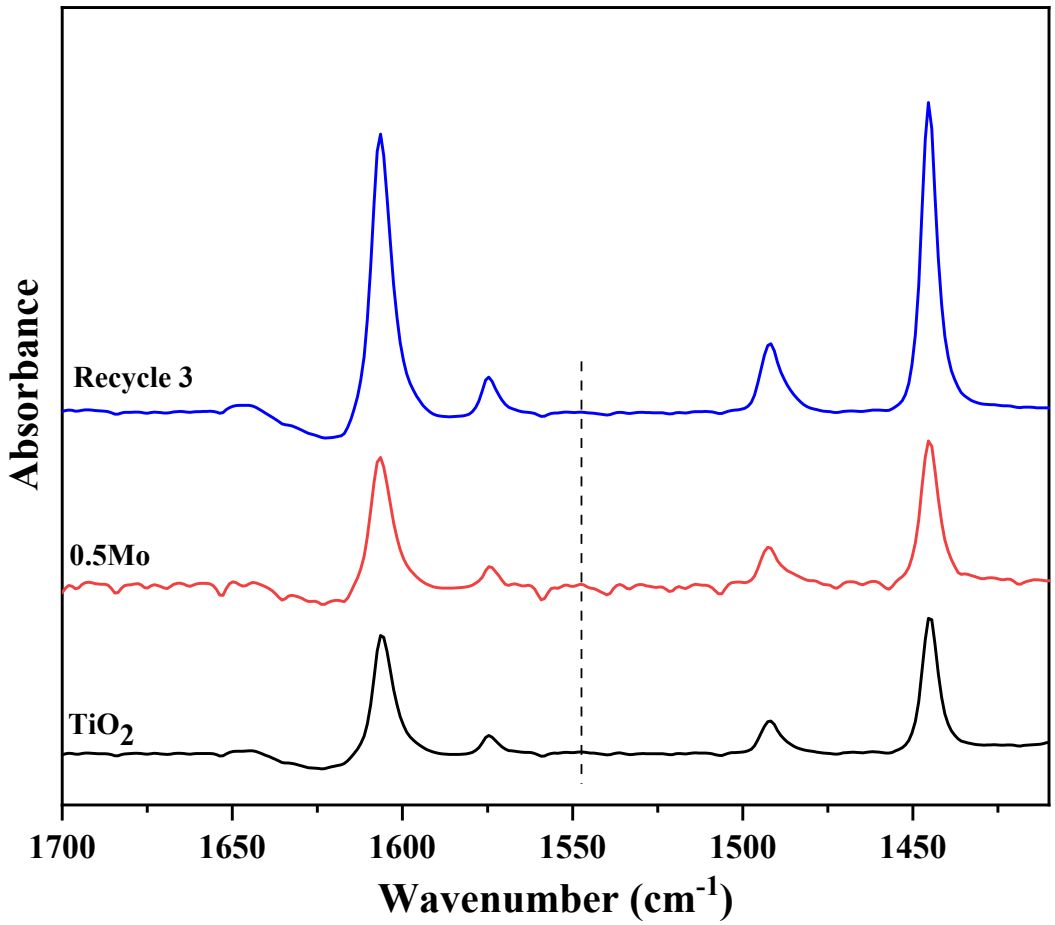


Fig. S9 Py-FTIR of TiO_2, 0.5Mo, and calcined recycle 3 catalysts showing the absence of Brønsted acid band at 1545 cm^{-1}.

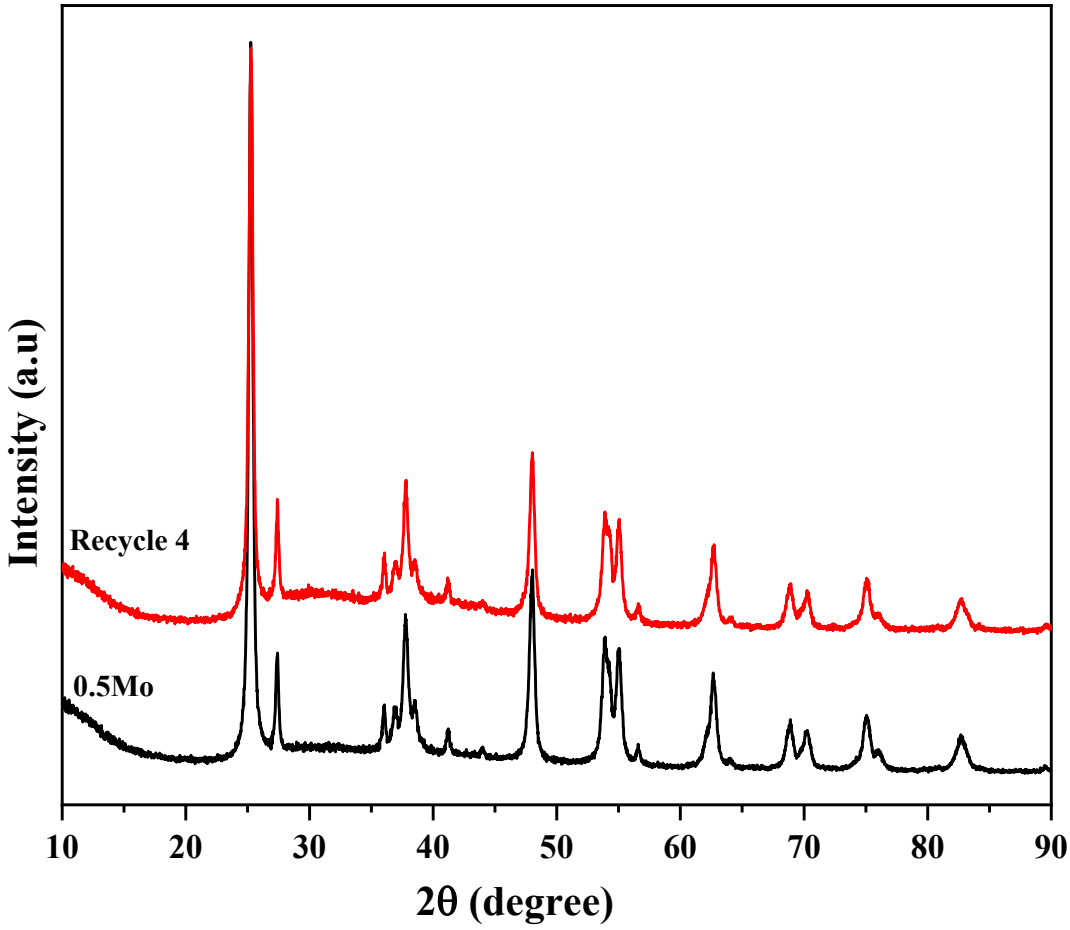


Fig. S10 XRD 0.5Mo and calcined recycle 4 catalysts.

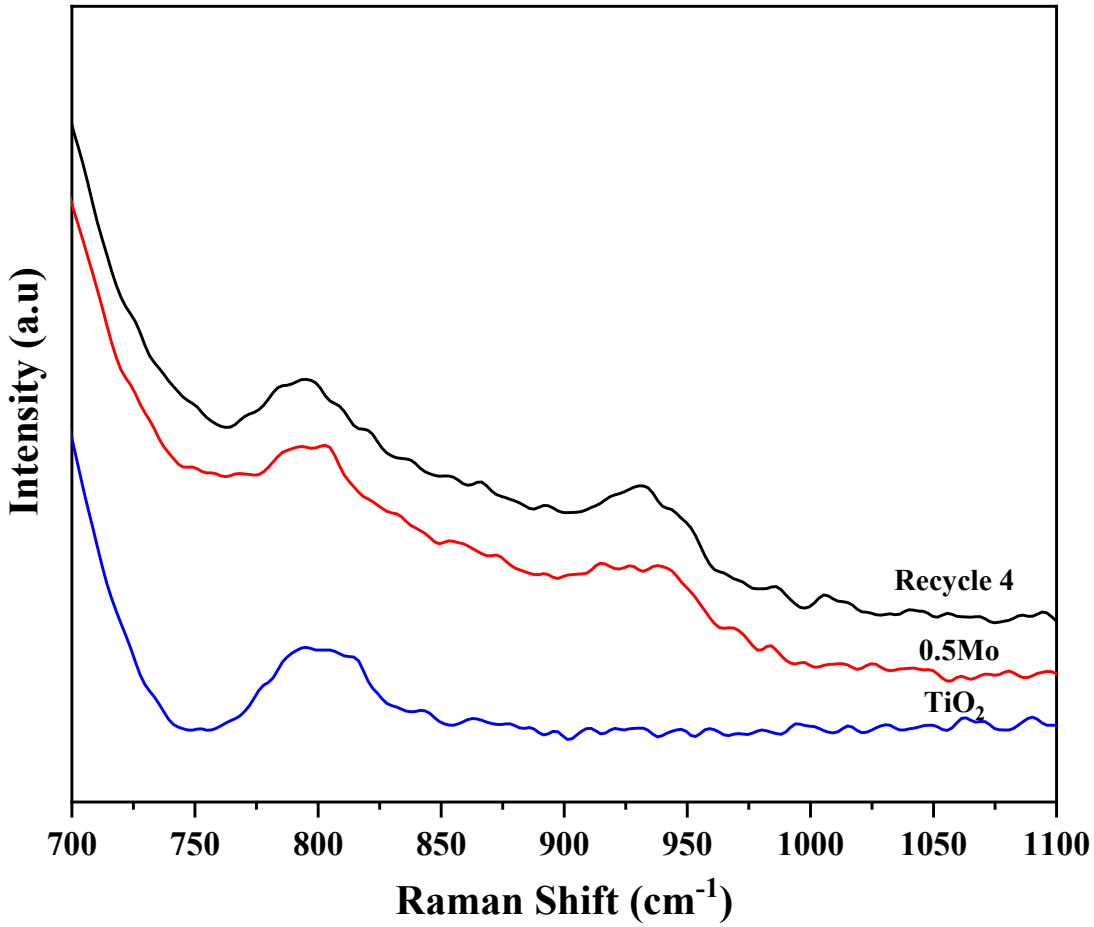
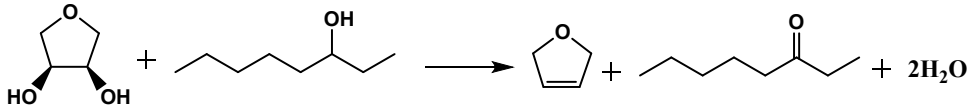
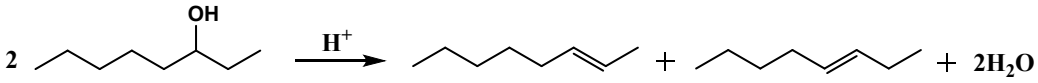


Fig. S11 Raman spectra of TiO_2, 0.5Mo, and calcined recycle 4 catalysts.

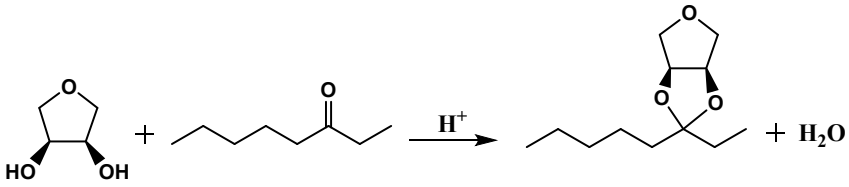
1. Desired reaction pathway



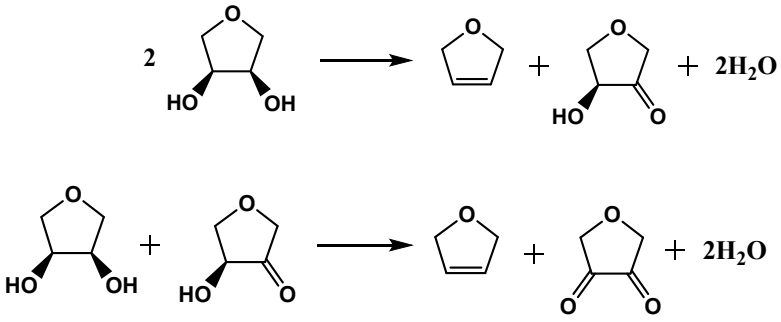
2. Dehydration of 3-octanol to 2-octene and 3-octene



3. Ketal formation from 1,4-AHE and 3-octanone



4. 1,4-AHE acting as sacrificial reducing agent



Scheme S1 Reaction pathways in the DODH of 1,4-AHE in the presence of 3-octanol.