Supplementary Information

Enhancement of *p*-Xylene Selectivity in the Reaction between 2,5-Dimethylfuran and Ethanol over Ammonium Fluoride Modified ZSM-5 Zeolite

Rongrong Zhao,*[a] Shikun Li,[b] Lixin Bi,[a] Qiang Fu,[a] Hongzi Tan,[a] Ming Wang,[a]and Hongyou Cui[a]

[a]*School of Chemical Engineering, Shandong University of Technology, 255091 Zibo, China*

[b] *Institute of Applied and Physical Chemistry, Faculty 02, University of Bremen,28359 Bremen, Germany*

*Corresponding author E-mail:rrzhao1990@sdut.edu.cn (R.Zhao)

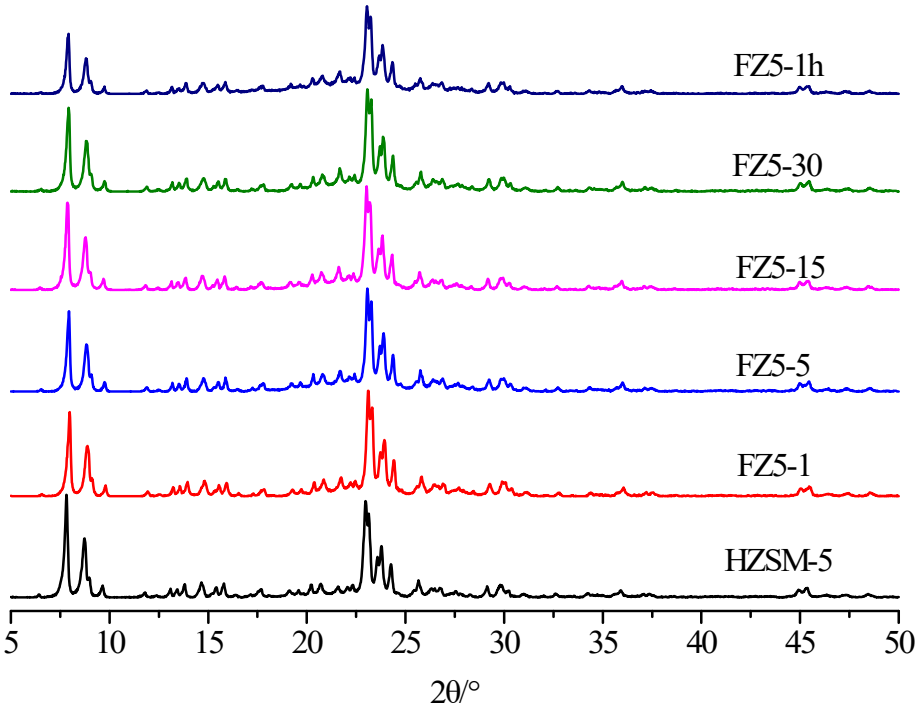


Figure S1 XRD patterns of various samples

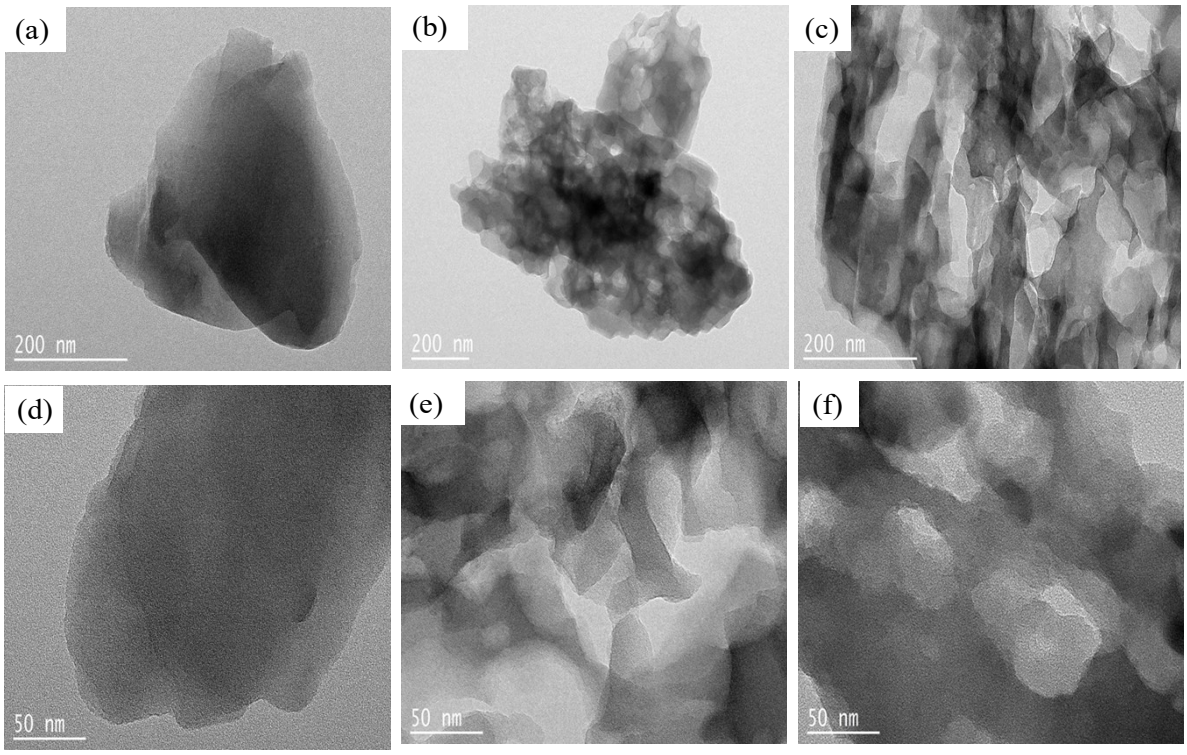


Figure S2 TEM images of various catalysts (a) HZSM-5,(b) FZ5-5, (c) FZ5-15

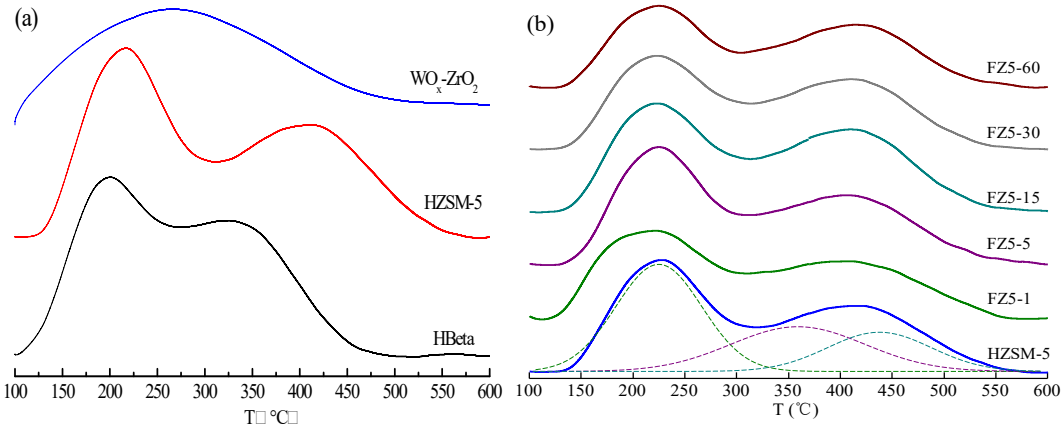
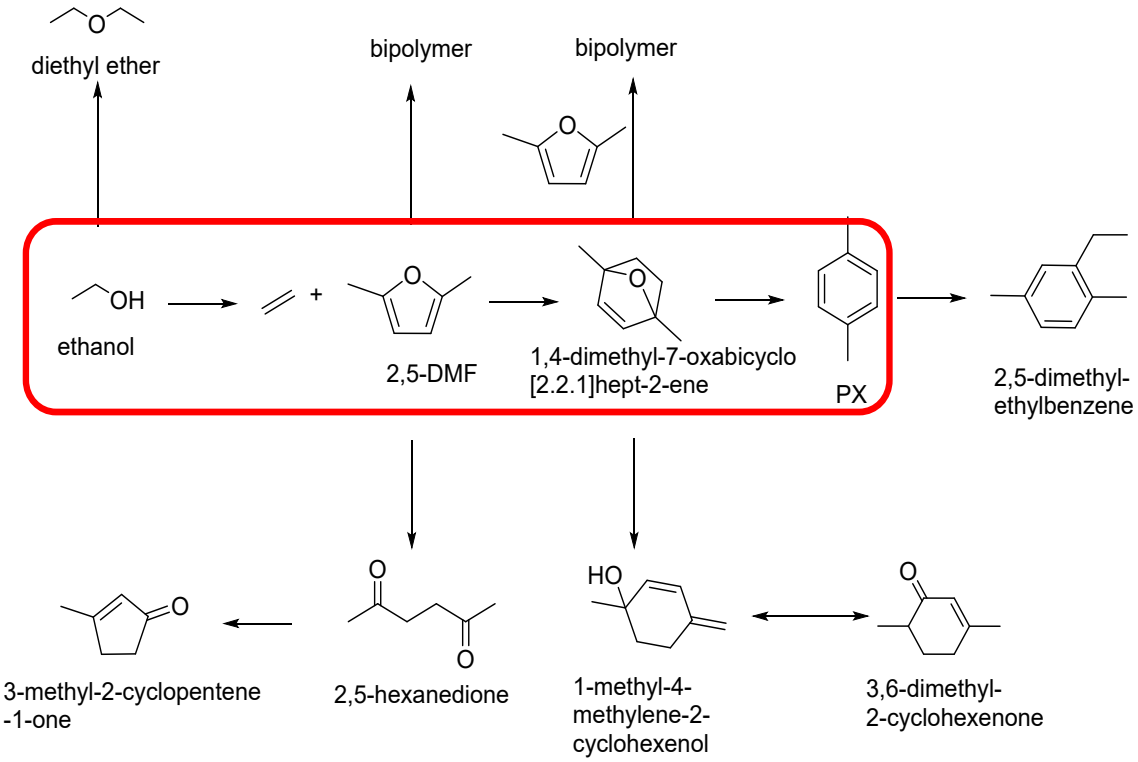


Figure S3 NH_3-TPD profiles of various catalyst (a) and HZSM-5 zeolite by NH_4F treatment (b)



Scheme S1 Reaction network between 2,5-DMF and ethanol

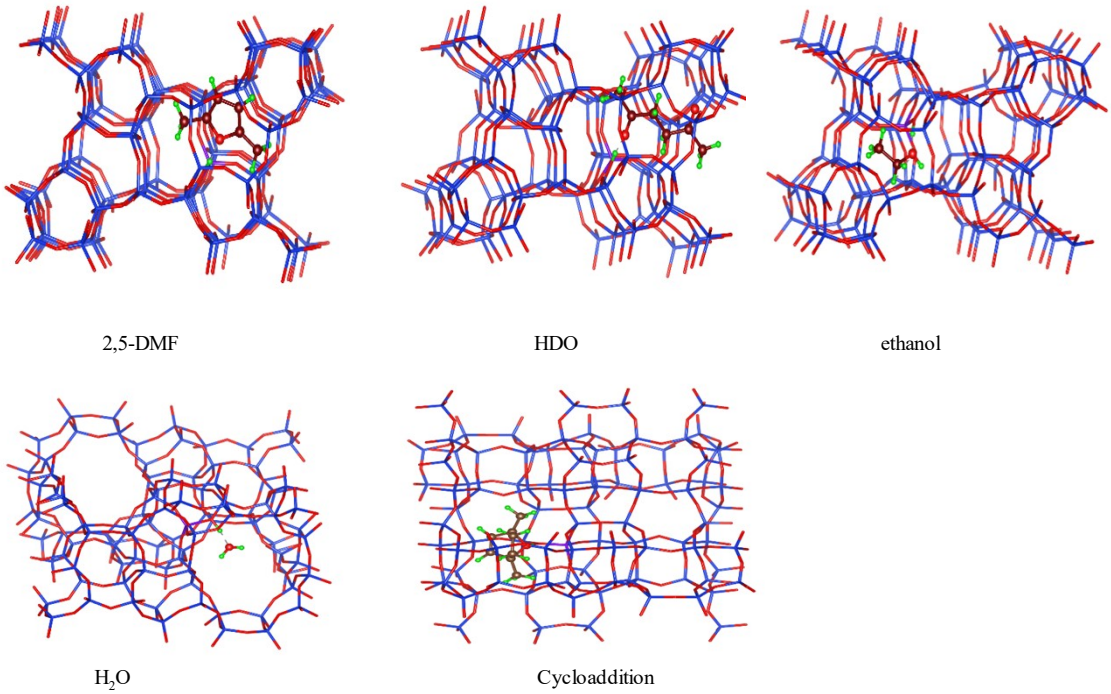


Figure S4 Optimized structure of reactants and products adsorbed in the pores of ZSM-5.C,O,Si, Al and H atoms are depicted as brown, red,blue,purple and green.

Table S1 Adsorption energies of several molecules on the acidic site of ZSM-5 zeolite

Adsorption energy	kJ/mol
MCO	111.873
ethanol	88.9124
H_2O	83.942
2,5-HDO	79.9205
cycloaddition	0.94843
DMF	-2.7

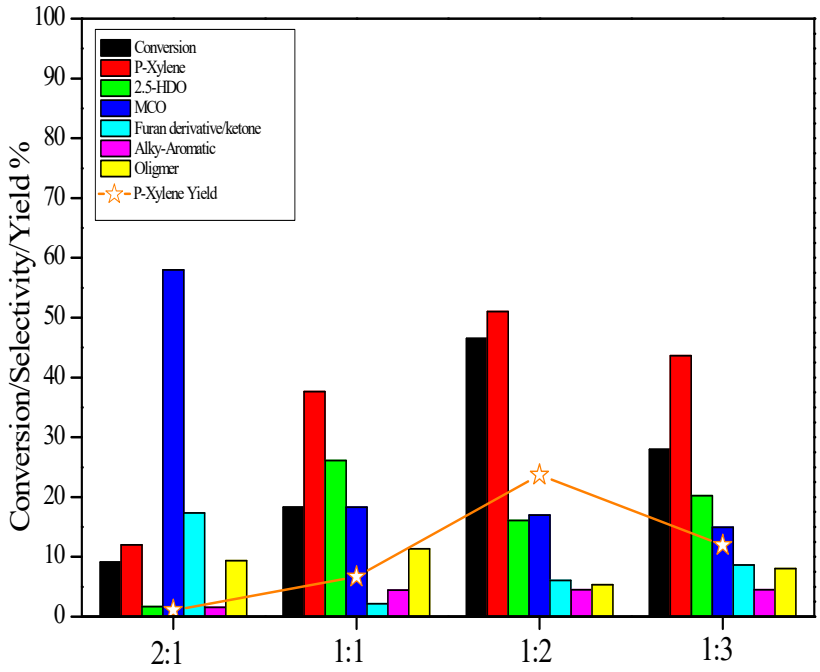


Figure S5 Catalytic performance for DMF reaction with ethanol over HBeta zeolite with different molar ratios DMF/ethanol.Reaction conditions: 3.75M reactant (DMF+ethanol) in heptane; temperature 300 °C; reaction time 12 h; 0.4 g catalyst.

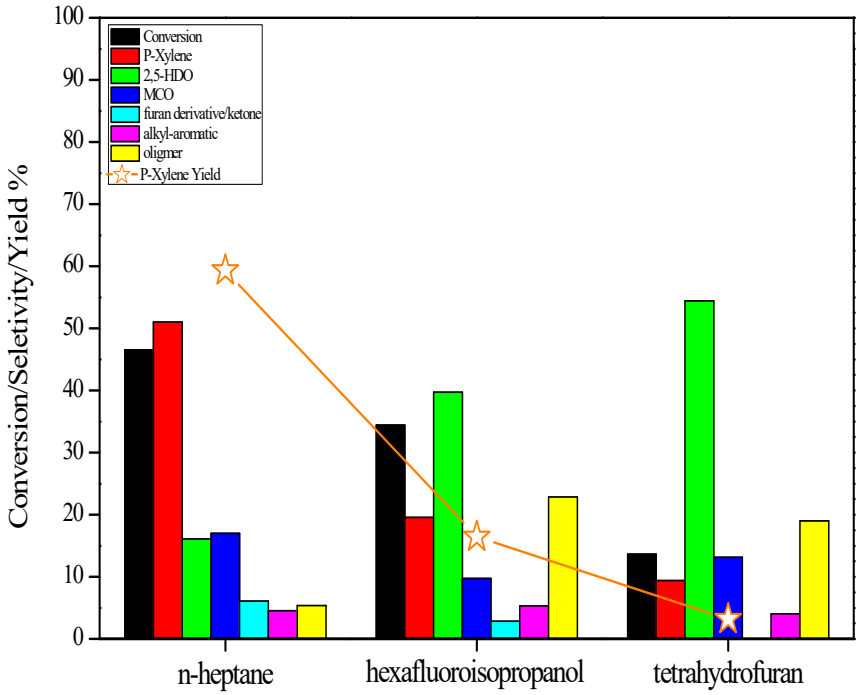


Figure S6 Catalytic performance for DMF reaction with ethanol over HBeta zeolite under various solvents.Reaction conditions: 3.75M reactant (DMF+ethanol) in solvent; temperature 300 °C; reaction time 12 h; 0.4 g catalyst.