A Surface Modification Strategy to Prepare Hierarchical Beta Molecular Sieves for Glucose Dehydration

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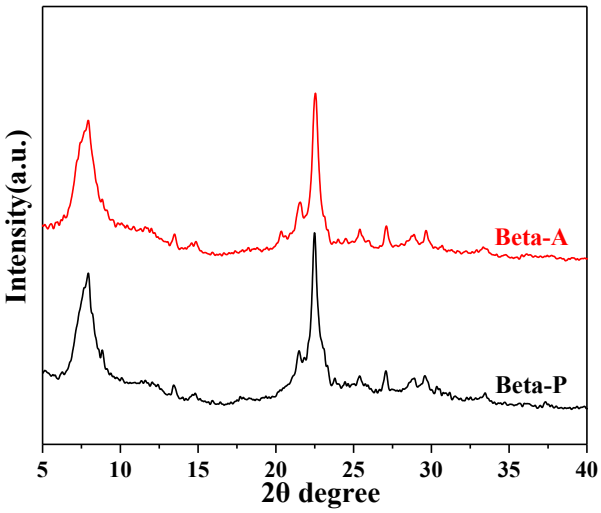

Fig. S1. XRD patterns of Beta-P and Beta-A.

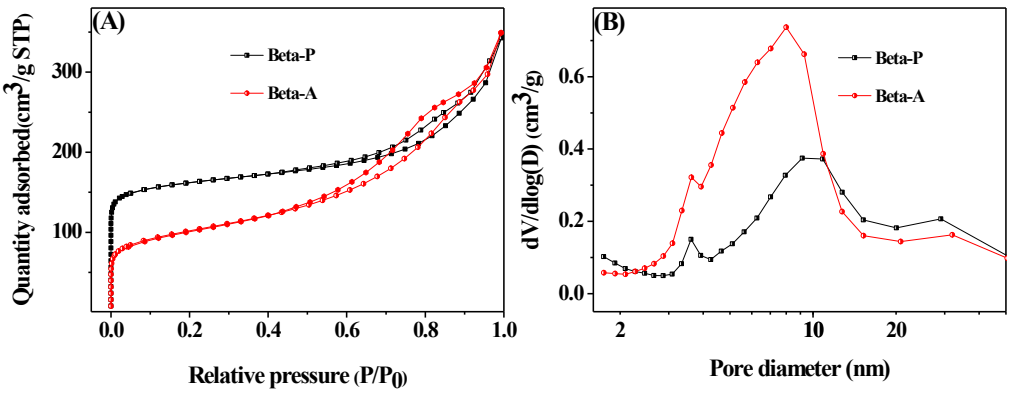

Fig. S2. N_2 adsorption-desorption isotherms (A) and BJH pore width distribution curves (B) of Beta-P and Beta-A. These data were obtained from previous published research. The DOI of previous research: 10.1039/d1cy00019e.

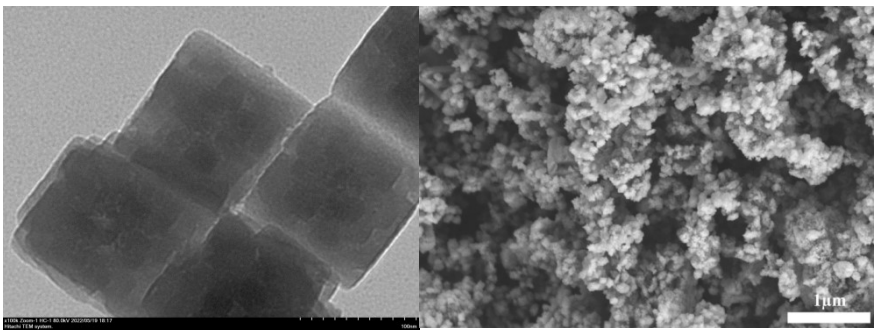

Fig. S3. TEM (left) and SEM (right) images of Beta-P.

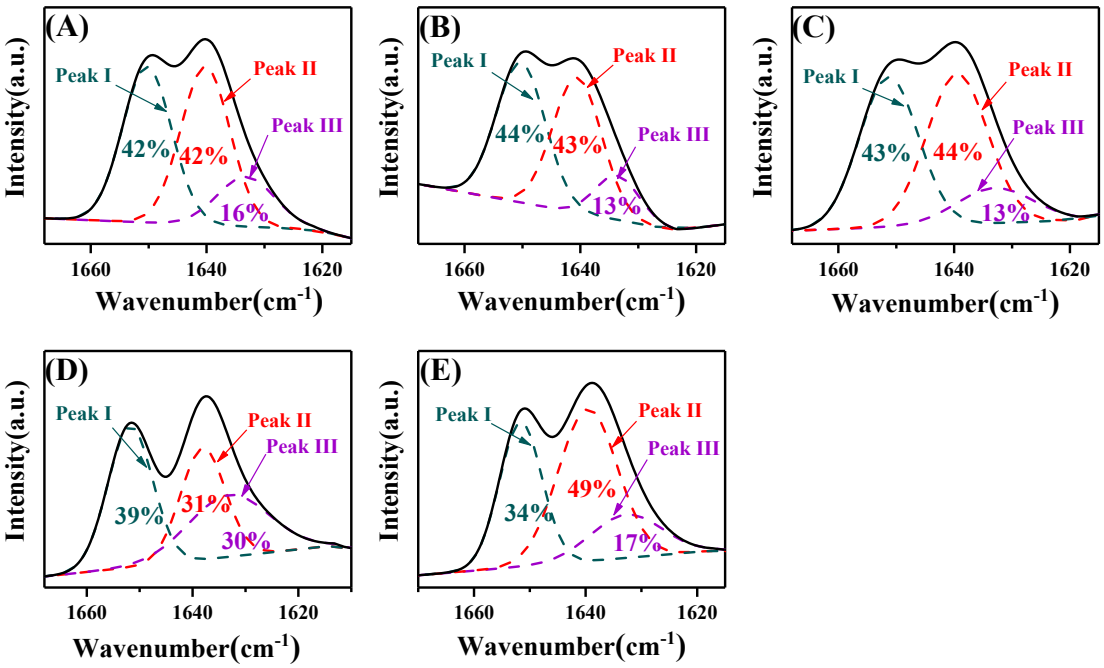

Fig. S4. Fitting results of collidine adsorbed FTIR spectra of Beta-PyC (A), Beta-DPyC (B), Beta-TPyC (C), Beta-P (D), and Beta-A (E).

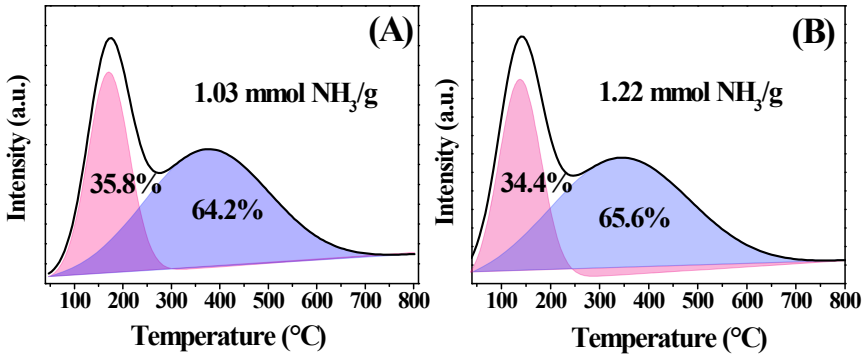

Fig. S5. Fitted NH_3-TPD spectra of Beta-P (A) and Beta-A (B). The total amount of acid sites is inserted in figures. Weak and strong acid sites are defined based on the desorption temperature of NH_3. When desorption temperature is <300 °C and > 300 °C, corresponding acid sites are weak and strong acid sites, respectively. These data were obtained from our previous research. DOI number is 10.1016/j.fuel.2022.123534.

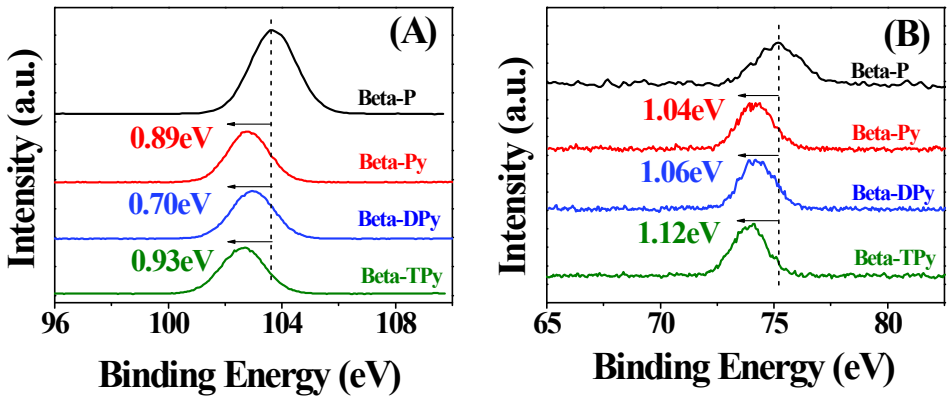

Fig. S6. Si2P (A) and Al2P (B) XPS of Beta, Beta-Py, Beta-DPy, and Beta-TPy.

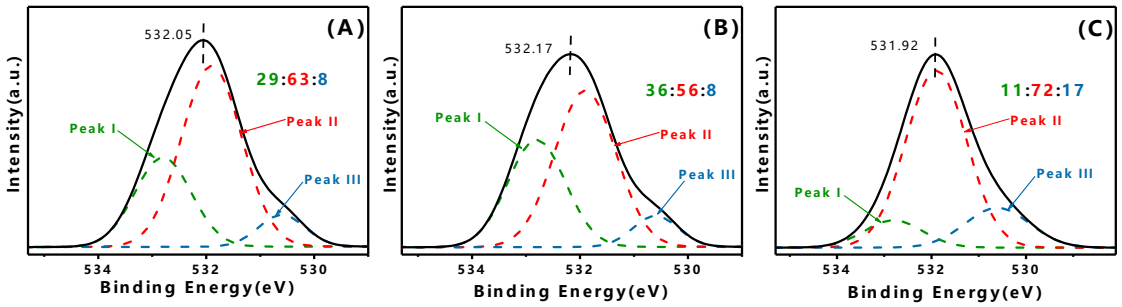

Fig. S7. Fitting results of the O1s XPS spectra of Beta-Py (A), Beta-DPy (B) and Beta-TPy (C).

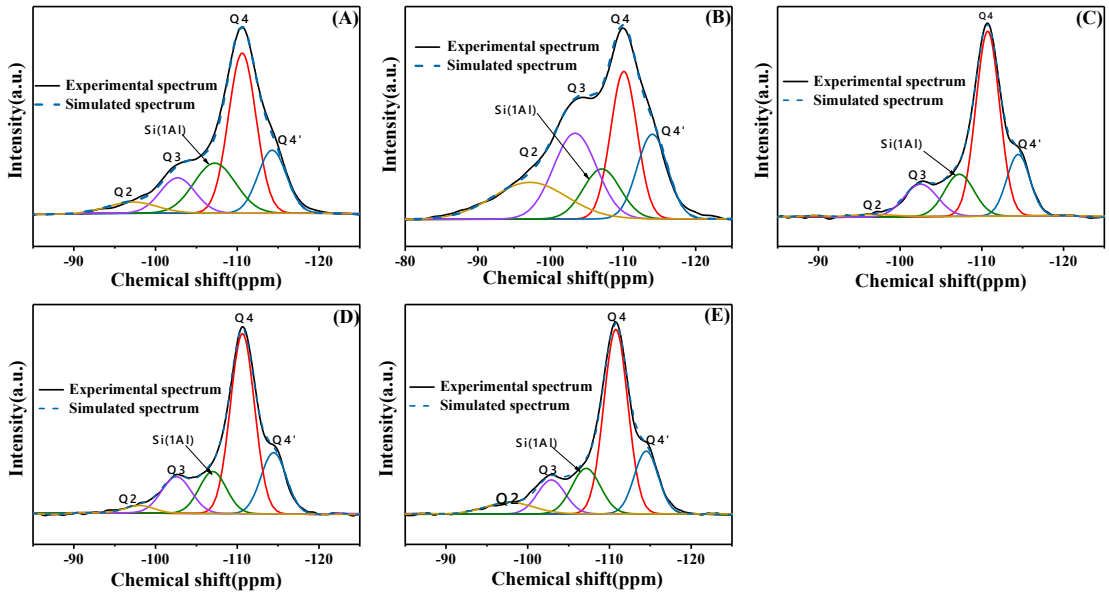

Fig. S8. ^{29}Si MAS NMR spectra and fitted curves of Beta-P (A), Beta-A(B), Beta-PyC (C), Beta-DPyC (D), And Beta-TPyC (E): Q_2, $(SiO)_2Si(OH)_2$; Q_3, $(Si)_3SiOH$; Si(1Al), $Si(OSi)_3(OAl)$; Q_4, $Si(OSi)_4$, and Q_4', the crystallographically inequivalent $Si(OSi)_4$ site[1].

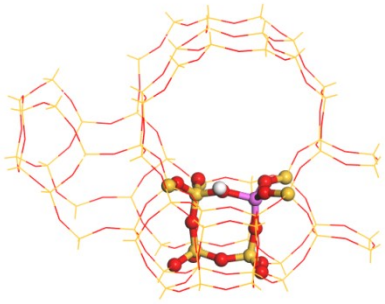

Fig. S9. Optimized topology structure of Beta molecular sieves.

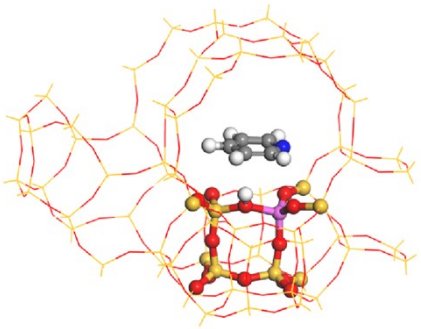

Fig. S10. Adsorption of pyridine molecules on Beta molecular sieves via an interaction between pyridine ring and bridge hydroxyl group.

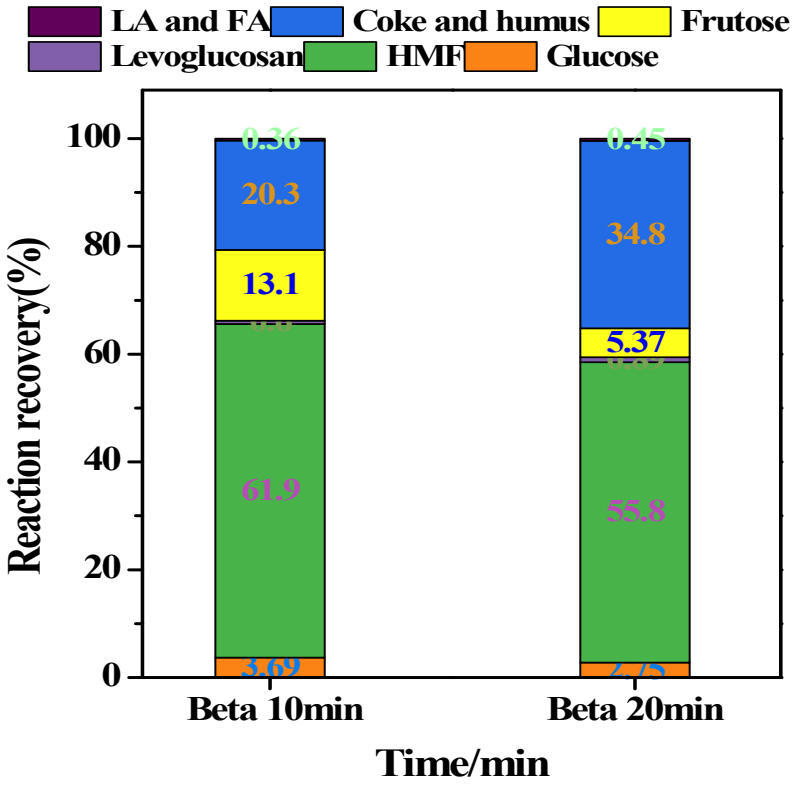

Fig. S11. Product distribution of dehydration reaction of glucose using Beta-P at 150 ℃ for 10 to 20min.

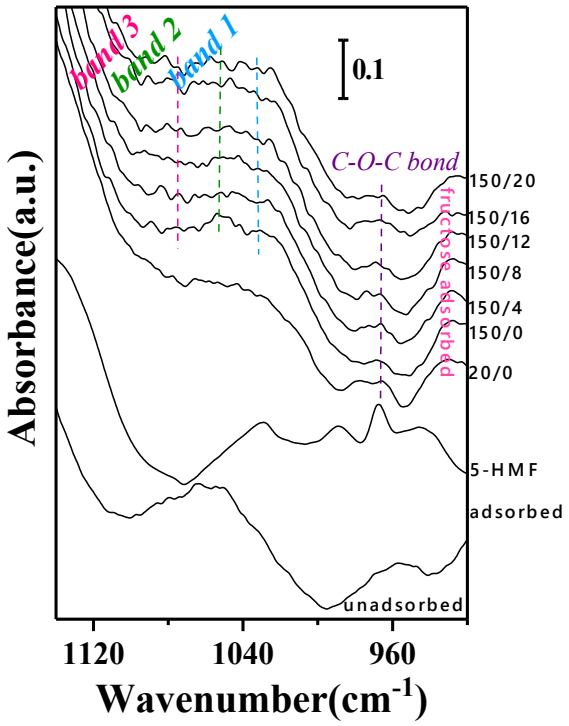

Fig. S12. ***In-situ*** **FTIR spectra of fructose dehydration on Beta-P.**

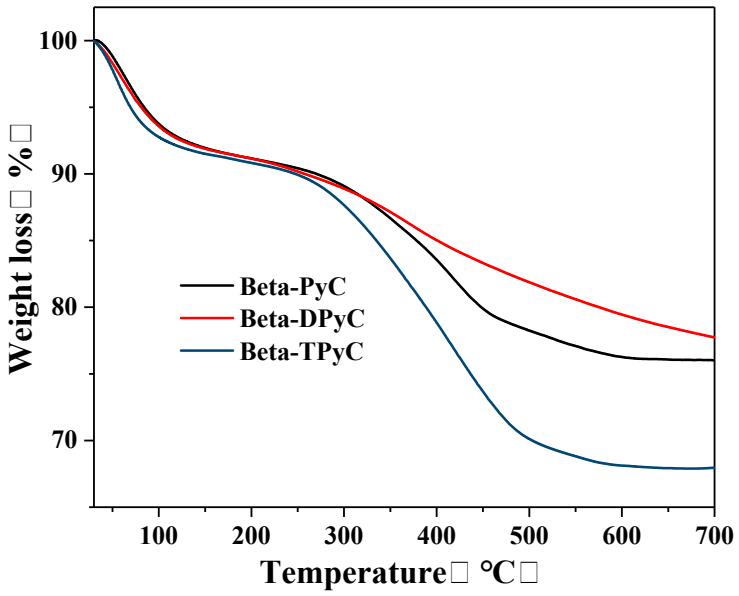

Fig. S13. TG analyzes the carbon deposition of Beta-PyC, Beta-DPyC and Beta-TPyC.

Table S1. Mulliken charge of atoms.

Cluster	Charge (e)								
	Al	Si1	Si2	Si3	Si4	O1	O2	O3	O4
Beta-P	2.031	2.381	2.370	2.368	2.353	-1.051	-1.243	-1.261	-1.247
Beta-PyC	2.022	2.357	2.359	2.353	2.358	-1.288	-1.248	-1.258	-1.251
Beta-DPyC	2.033	2.357	2.358	2.352	2.353	-1.296	-1.244	-1.255	-1.250
Beta-TPyC	2.036	2.394	2.377	2.381	2.358	-1.056	-1.242	-1.258	-1.252

Table S2. Length of Si-O and Al-O bonds.

Cluster	Bond length (nm)							
	Al-O1	Al-O2	Al-O3	Al-O4	Si1-O1	Si2-O2	Si3-O3	Si4-O4
Beta-P	1.900	1.682	1.697	1.683	1.702	1.593	1.595	1.581
Beta-PyC	1.757	1.714	1.723	1.693	1.598	1.590	1.584	1.579
Beta-DPyC	1.757	1.710	1.725	1.698	1.597	1.589	1.579	1.580
Beta-TPyC	1.894	1.686	1.692	1.684	1.695	1.591	1.591	1.583

1. D. Xiao, S. Xu, N. J. Brownbill, S. Paul, L. H. Chen, S. Pawsey, F. Aussenac, B. L. Su, X. Han, X. Bao, Z. Liu and F. Blanc, Fast detection and structural identification of carbocations on zeolites by dynamic nuclear polarization enhanced solid-state NMR, *Chem Sci*, 2018, **9**, 8184-8193.