Supporting Information

Synergy between Lewis acid sites and hydroxyl groups for the isomerization of glucose to fructose over Sn-containing zeolites: a theoretical perspective

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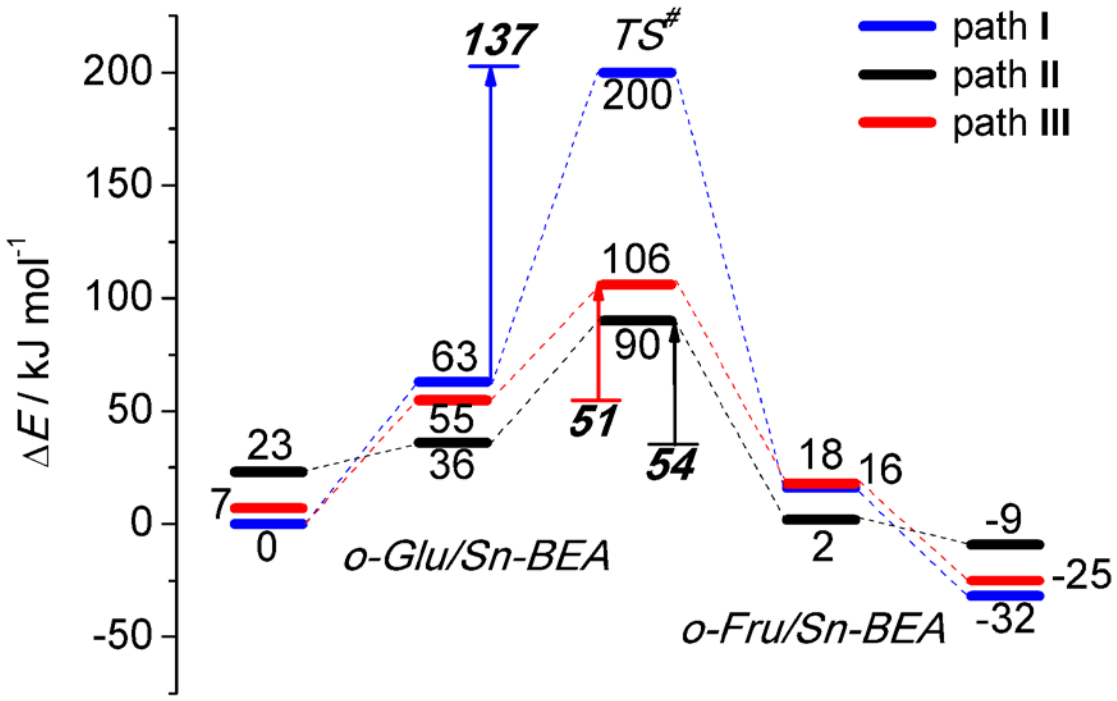


Figure S1. DFT computed reaction energy diagram of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-BEA without *vdW* correction.

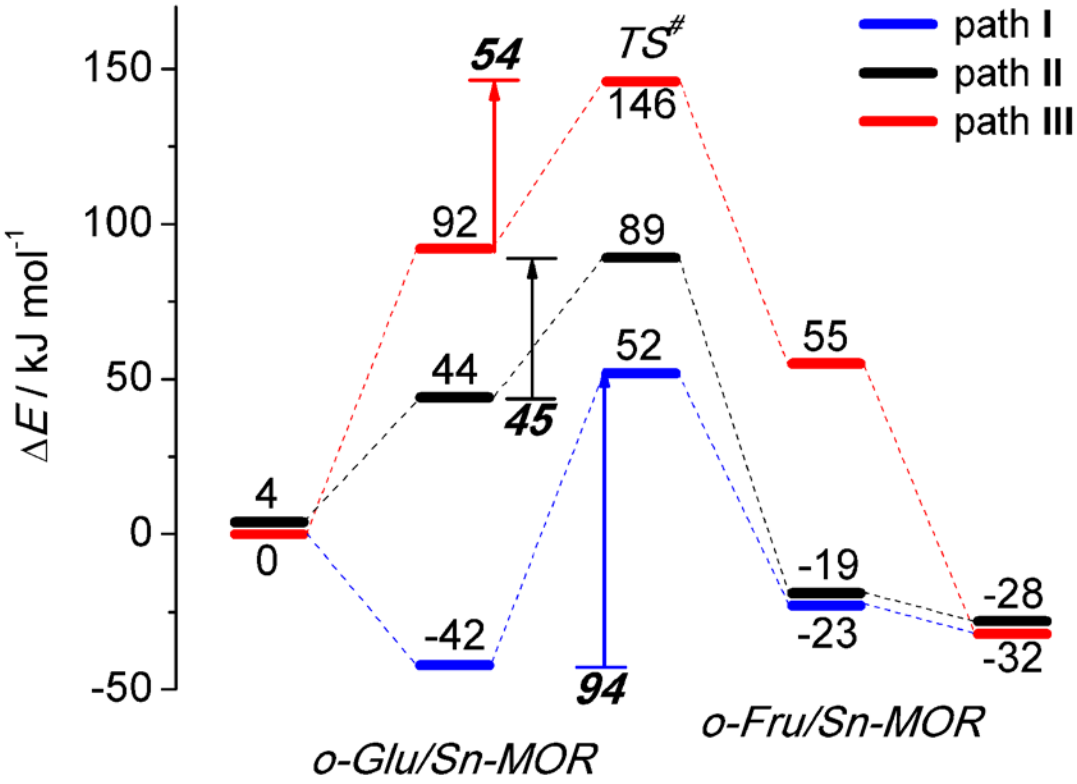


Figure S2. DFT computed reaction energy diagram of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MOR without *vdW* correction.

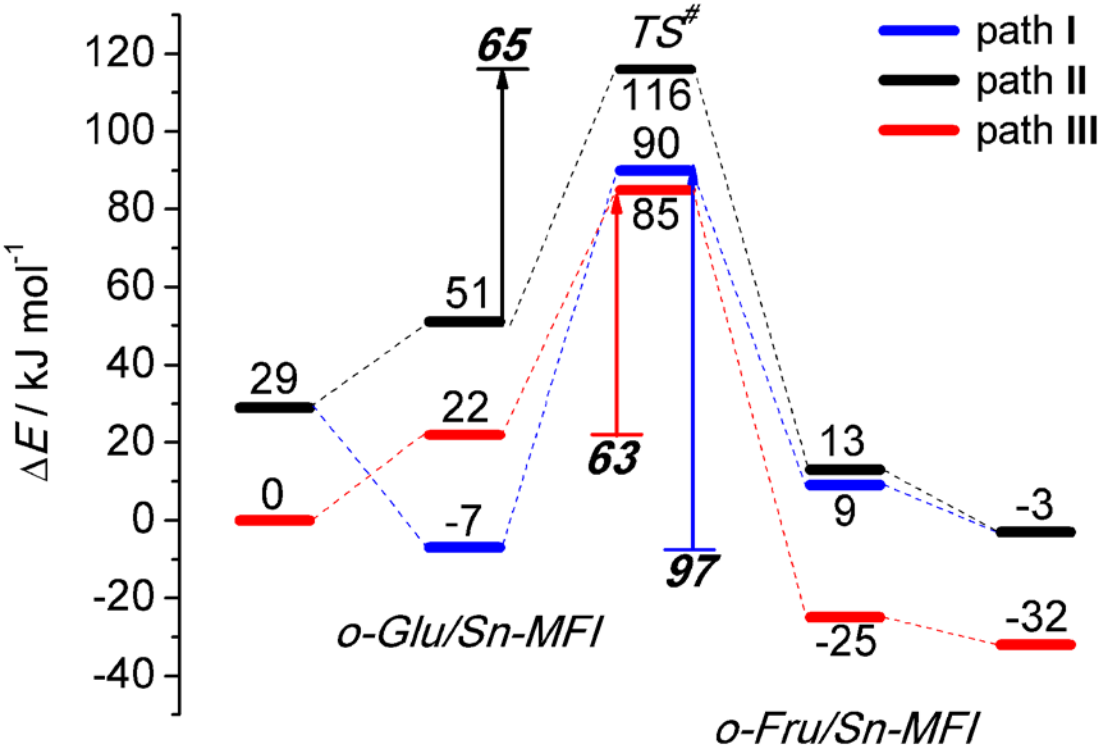


Figure S3. DFT computed reaction energy diagram of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MFI without *vdW* correction.

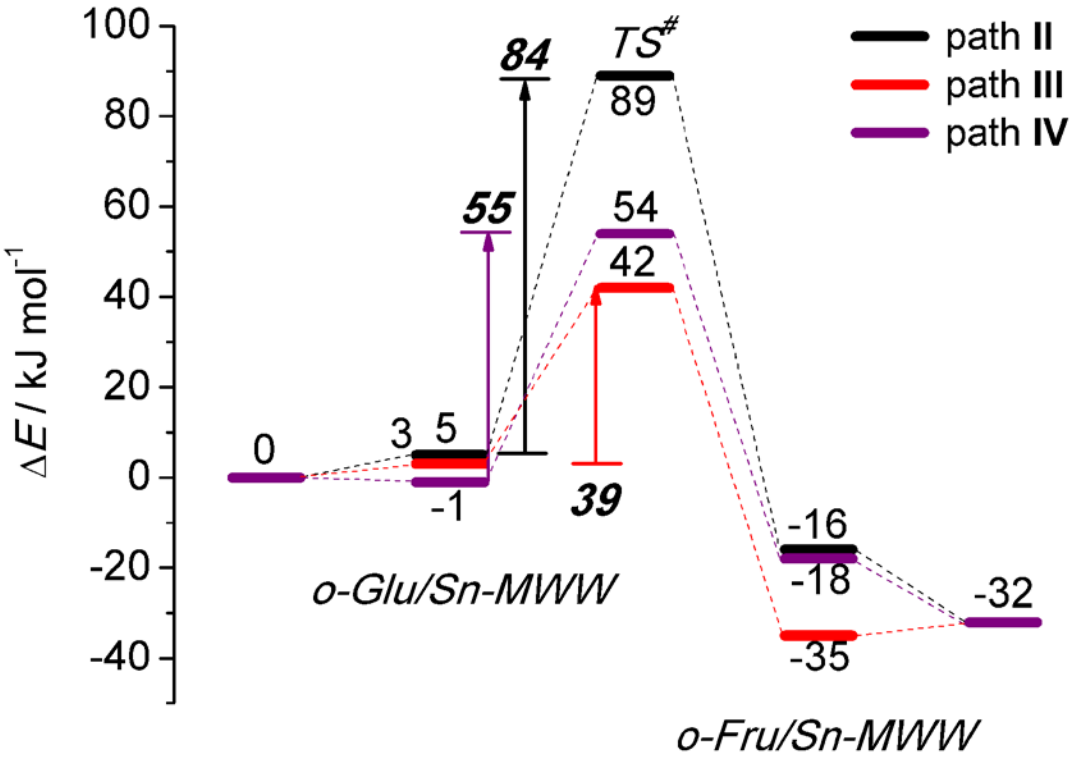


Figure S4. DFT computed reaction energy diagram of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MWW without *vdW* correction.

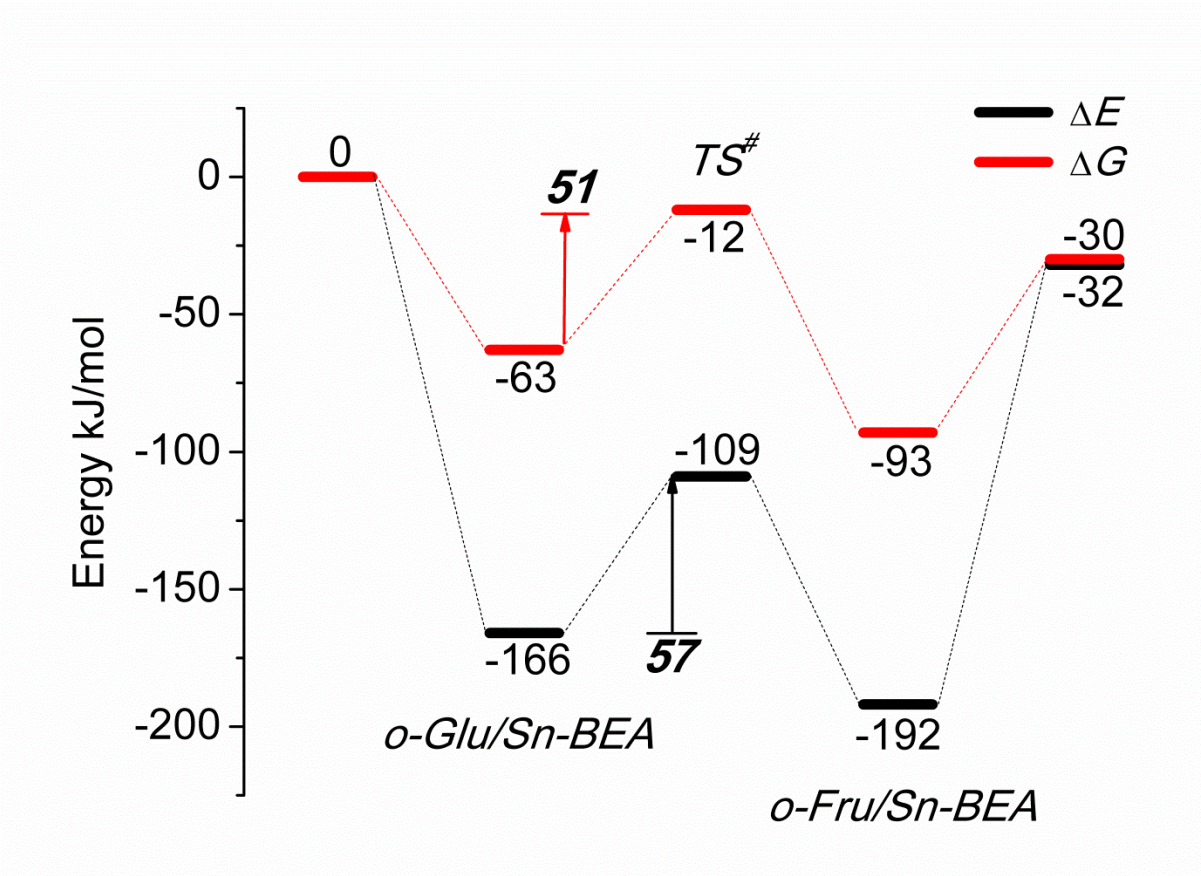


Figure S5. Reaction free energy (*T* = 373K) and DFT-D2 energy of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-BEA (path **II**).

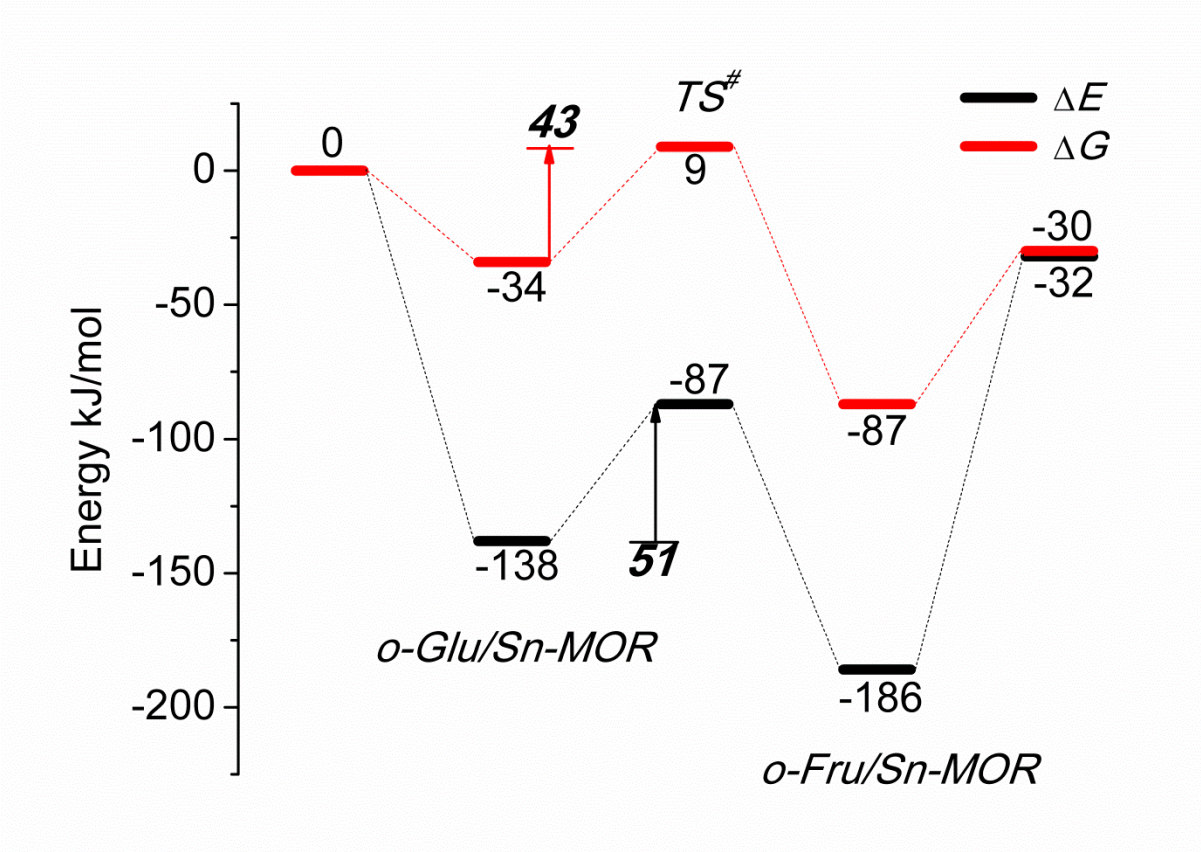


Figure S6. Reaction free energy (*T* = 373K) and DFT-D2 energy of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MOR (path **II**).

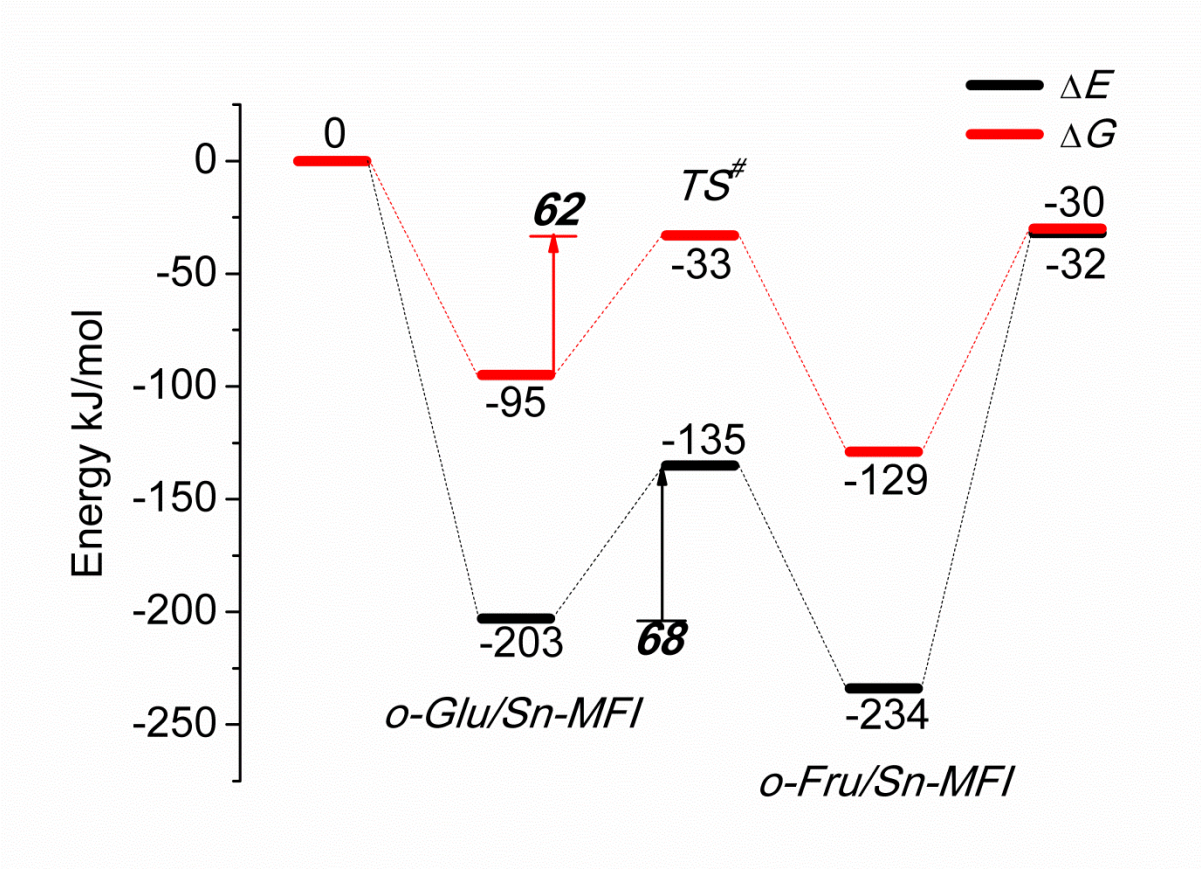


Figure S7. Reaction free energy (*T* = 373K) and DFT-D2 energy of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MFI (path **II**).

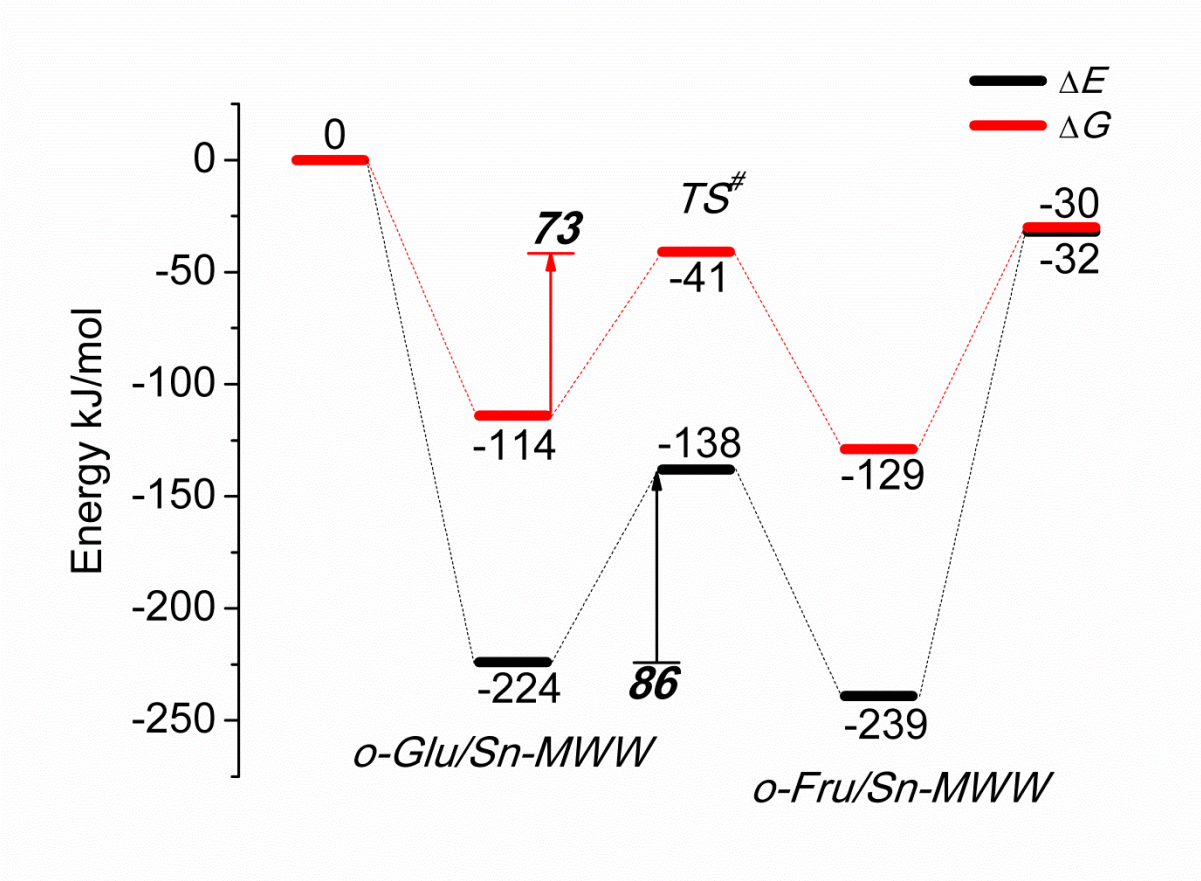


Figure S8. Reaction free energy (*T* = 373K) and DFT-D2 energy of o-*Glu* isomerization to o-*Fru* over SnOH site of Sn-MWW (path **II**).

Table S1. Optimized unit cell lattice parameters of selected zeolites in their all-silica forms.

Zeolite	Lattice parameters
MOR	$a = b = 13.65$ Å, $c = 15.02$ Å, $\gamma = 97°$
BEA	$a = b = 12.66$ Å, $c = 26.40$ Å, $\alpha = \beta = \gamma = 90°$
MFI	$a = 20.12$ Å, $b = 19.77$ Å, $c = 13.16$ Å, $\alpha = \beta = \gamma = 90°$
MWW	$a = b = 14.11$ Å, $c = 24.88$ Å, $\gamma = 120°$

Table S2. Bader Charge analysis of selected atoms in reaction path **I**.

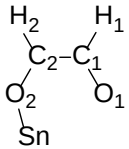
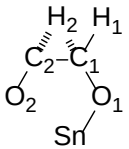
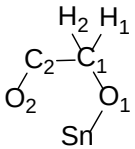
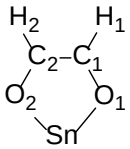
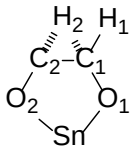
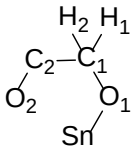
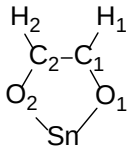
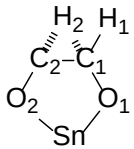
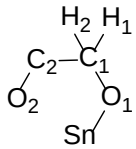
Bader Charge/e	*Beta*			*MFI*			*MOR*		
									
	a-Glu	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-Fru*
C2	0,48	0,70	0,95	0,46	0,64	0,86	0,39	0,46	0,79
C1	0,96	0,64	0,42	0,86	0,57	0,28	0,82	0,72	0,37
O2	-1,10	-1,15	-1,10	-1,04	-1,09	-1,09	-1,08	-1,09	-1,10
O1	-1,05	-1,14	-1,11	-1,05	-1,08	-0,98	-1,06	-1,06	-1,05
H2	0,03	0,09	0,07	0,11	0,12	0,15	0,15	0,10	0,13
H1	0,05	0,14	0,12	0,17	0,21	0,14	0,19	0,19	0,16
Sn	2,36	2,35	2,35	2,31	2,32	2,31	2,29	2,29	2,29

Table S3. Bader Charge analysis of selected atoms in reaction path **II**.

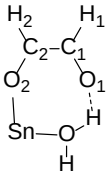
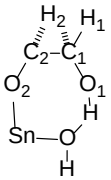
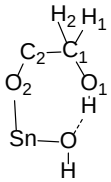
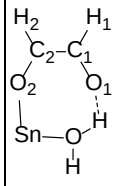
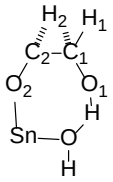
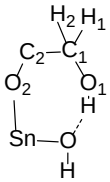
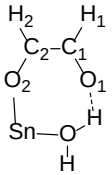
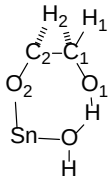
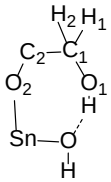
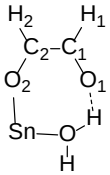
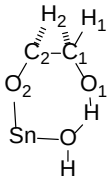
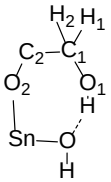
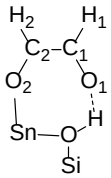
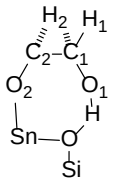
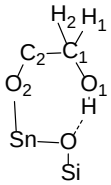
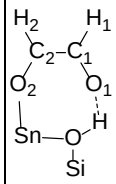
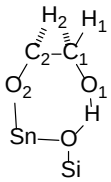
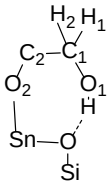
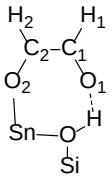
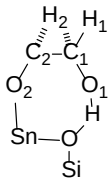
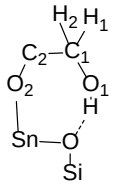
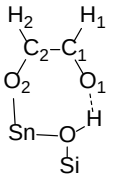
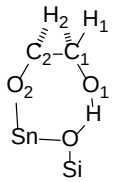
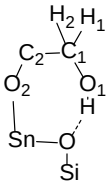
Bader charge/e	*Beta*			*MFI*			*MOR*			*MWW*		
												
	a-Glu	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-fru*	*a-Glu*	*TS*	*a-fru*
C2	0,49	0,65	0,91	0,43	0,64	0,99	0,42	0,67	0,91	0,43	0,63	0,88
C1	0,88	0,64	0,50	0,83	0,61	0,26	0,88	0,74	0,45	0,78	0,71	0,38
O2	-1,16	-1,15	-1,08	-1,05	-1,13	-1,15	-1,09	-1,15	-1,11	-1,07	-1,14	-1,11
O1	-1,07	-1,18	-1,12	-1,05	-1,16	-1,16	-1,08	-1,16	-1,22	-1,04	-1,15	-1,26
H2	0,11	0,09	0,08	0,09	0,10	0,12	0,12	0,10	0,06	0,12	0,11	0,11
H1	0,06	0,18	0,04	0,15	0,20	0,22	0,07	0,05	0,10	0,17	0,13	0,15
Sn	2,37	2,36	2,30	2,36	2,38	2,33	2,32	2,32	2,32	2,38	2,37	2,36
O_{H2O}	-1,34	-1,28	-1,29	-1,36	-1,26	-1,26	-1,35	-1,38	-1,21	-1,38	-1,32	-1,45
H_{H2O}	0,69	0,70	0,63	0,71	0,72	0,67	0,69	0,68	0,72	0,69	0,66	0,78

Table S4. Bader Charge analysis of selected atoms in reaction path **III**.

Bader charge/e	*Beta*			*MFI*			*MOR*			*MWW*		
												
	a-Glu	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-Fru*	*a-Glu*	*TS*	*a-fru*	*a-Glu*	*TS*	*a-fru*
C2	0,50	0,75	0,92	0,51	0,74	0,85	0,50	0,69	0,86	0,58	0,71	0,89
C1	0,80	0,56	0,47	0,88	0,54	0,40	0,89	0,62	0,36	0,74	0,57	0,44
O2	-1,15	-1,16	-1,12	-1,11	-1,14	-1,15	-1,12	-1,15	-1,10	-1,08	-1,13	-1,13
O1	-1,08	-1,22	-1,18	-1,09	-1,47	-1,15	-1,08	-1,12	-1,23	-1,13	-1,24	-1,18
H2	0,10	0,09	0,08	0,07	0,10	0,17	0,10	0,12	0,11	0,11	0,13	0,14
H1	0,14	0,21	0,06	0,09	0,19	0,09	0,06	0,15	0,14	0,18	0,23	0,10
Sn	2,40	2,39	2,37	2,35	2,40	2,39	2,35	2,35	2,35	2,33	2,35	2,35
$_{Si}O_{H}$	-1,42	-1,38	-1,37	-1,44	-1,39	-1,38	-1,48	-1,40	-1,38	-1,36	-1,35	-1,35
$_{SiO}H$	0,69	0,74	0,71	0,70	1,00	0,64	0,72	0,66	0,73	0,73	0,76	0,68