Supporting Information

Intra-Crystalline Mesoporous Zeolite [Al,Zr]-Y for Catalytic Cracking

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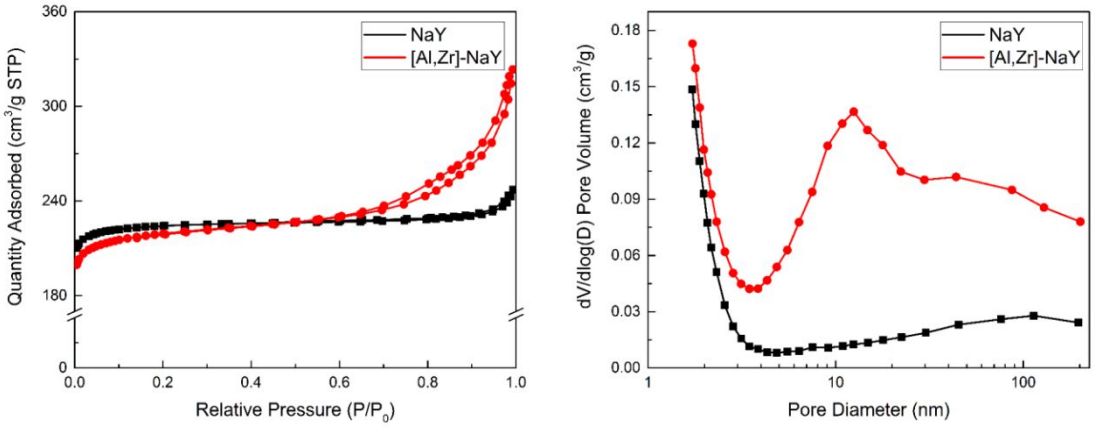

Figure S1. N_2 adsorption and desorption isotherms (left) and pore-size distributions (right) for NaY and [Al,Zr]-NaY zeolites.

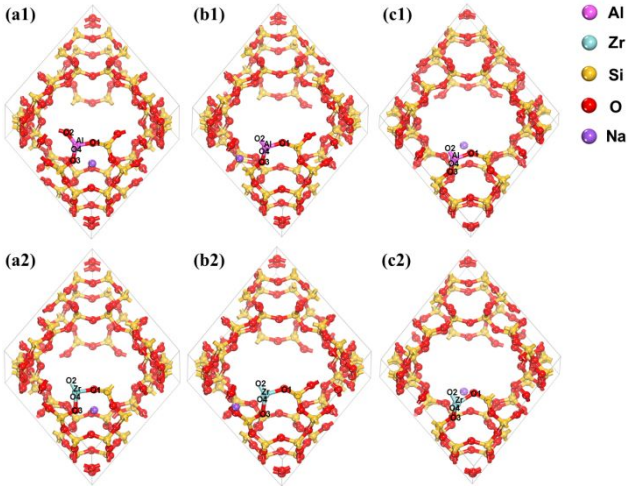

Figure S2. Optimized periodic Al-FAU and [Al,Zr]-FAU models for Na in (a) the α site, (b) the β site, and (c) the γ site.

Table S1. Bond lengths and angles for Al-FAU and [Al,Zr]-FAU with Na in the α sites

Al-FAU	Bond lengths (Å)	[Al,Zr]-FAU	Bond lengths (Å)	Al-FAU	Bond angles (°)	[Al,Zr]-FAU	Bond angles (°)
Al-O1	1.762	Zr-O1	2.082	O1-Al-O2	99.203	O1-Zr-O2	83.820
Al-O2	1.742	Zr-O2	2.076	O2-Al-O3	114.628	O2-Zr-O3	132.560
Al-O3	1.732	Zr-O3	2.010	O3-Al-O4	112.702	O3-Zr-O4	105.052
Al-O4	1.716	Zr-O4	1.992	O1-Al-O4	111.983	O1-Zr-O4	132.614
Si1-O1	1.600	Si1-O1	1.610	Al-O1-Si1	139.138	Zr-O1-Si1	119.740
Si2-O2	1.586	Si2-O2	1.608	Al-O2-Si2	136.591	Zr-O2-Si2	113.329
Si3-O3	1.598	Si3-O3	1.614	Al-O3-Si3	138.058	Zr-O3-Si3	124.818
Si4-O4	1.586	Si4-O4	1.607	Al-O4-Si4	134.020	Zr-O4-Si4	121.674

Table S2. Bond lengths and angles for Al-FAU and Zr-FAU with Na in the β sites

Al-FAU	Bond lengths (Å)	[Al,Zr]-FAU	Bond lengths (Å)	Al-FAU	Bond angles (°)	[Al,Zr]-FAU	Bond angles (°)
Al-O1	1.734	Zr-O1	2.030	O1-Al-O2	113.797	O1-Zr-O2	104.679
Al-O2	1.704	Zr-O2	1.998	O2-Al-O3	112.717	O2-Zr-O3	132.582
Al-O3	1.793	Zr-O3	2.111	O3-Al-O4	106.214	O3-Zr-O4	91.358
Al-O4	1.731	Zr-O4	2.027	O1-Al-O4	112.017	O1-Zr-O4	138.800
Si1-O1	1.579	Si1-O1	1.590	Al-O1-Si1	143.547	Zr-O1-Si1	130.291
Si2-O2	1.576	Si2-O2	1.603	Al-O2-Si2	142.084	Zr-O2-Si2	116.439
Si3-O3	1.615	Si3-O3	1.620	Al-O3-Si3	130.046	Zr-O3-Si3	122.416
Si4-O4	1.580	Si4-O4	1.594	Al-O4-Si4	130.875	Zr-O4-Si4	117.437

Table S3. Bond lengths and angles for Al-FAU and Zr-FAU with Na in the γ sites

Al-FAU	Bond lengths (Å)	[Al,Zr]-FAU	Bond lengths (Å)	Al-FAU	Bond angles (°)	[Al,Zr]-FAU	Bond angles (°)
Al-O1	1.709	Zr-O1	1.986	O1-Al-O2	113.619	O1-Zr-O2	108.428
Al-O2	1.757	Zr-O2	2.083	O2-Al-O3	109.860	O2-Zr-O3	119.565
Al-O3	1.728	Zr-O3	1.997	O3-Al-O4	112.346	O3-Zr-O4	104.193
Al-O4	1.779	Zr-O4	2.111	O1-Al-O4	109.977	O1-Zr-O4	113.036
Si1-O1	1.589	Si1-O1	1.605	Al-O1-Si1	140.495	Zr-O1-Si1	126.376
Si2-O2	1.601	Si2-O2	1.616	Al-O2-Si2	135.685	Zr-O2-Si2	109.920
Si3-O3	1.599	Si3-O3	1.617	Al-O3-Si3	135.961	Zr-O3-Si3	130.353
Si4-O4	1.613	Si4-O4	1.617	Al-O4-Si4	127.029	Zr-O4-Si4	118.120

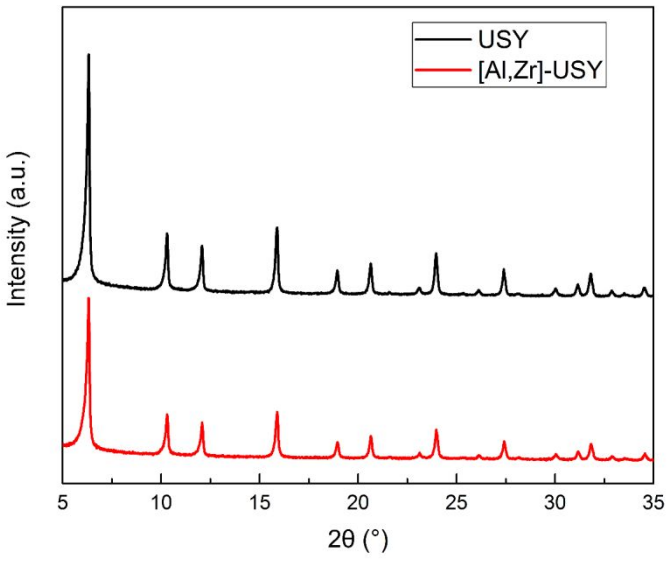

Figure S3. XRD patterns of USY and [Al,Zr]-USY.

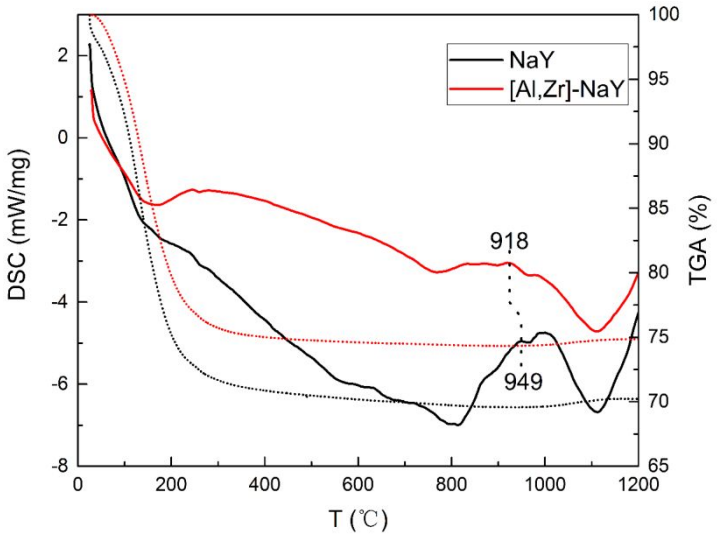

Figure S4. DSC and TGA curves for the NaY and [Al,Zr]-NaY zeolites

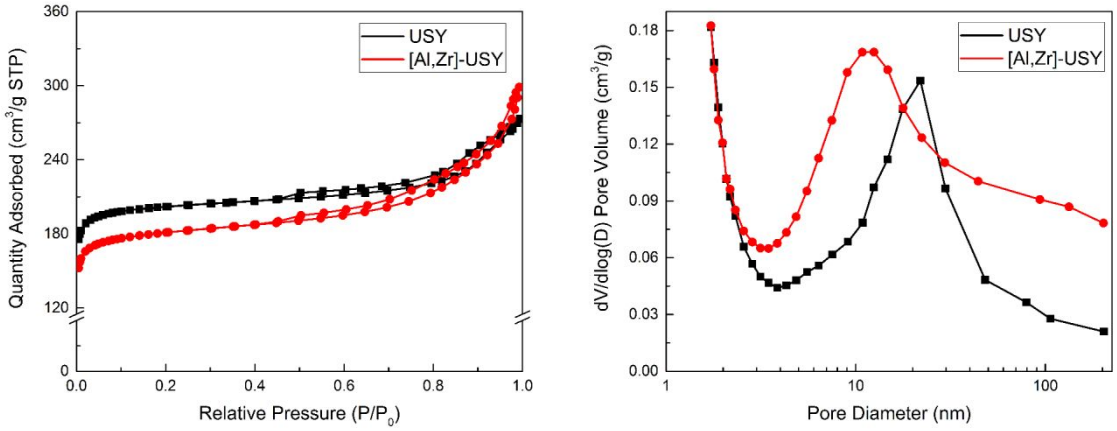

Figure S5. N_2 adsorption and desorption isotherms and pore-size distributions of zeolites.

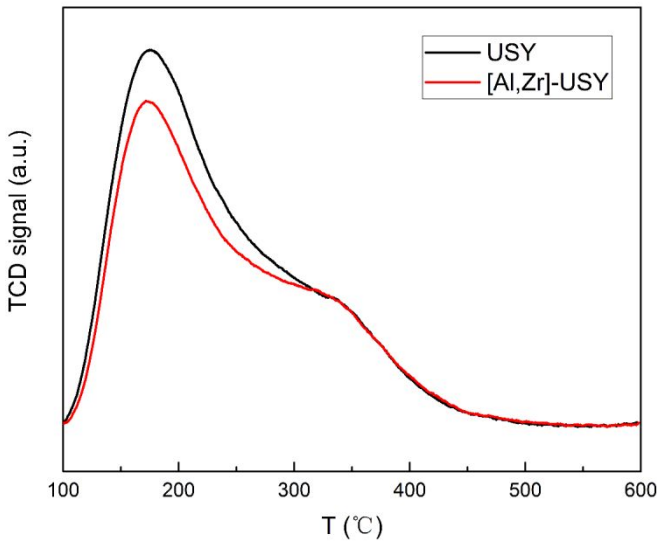

Figure S6. NH_3-TPD profiles of the USY and [Al,Zr]-USY zeolites.

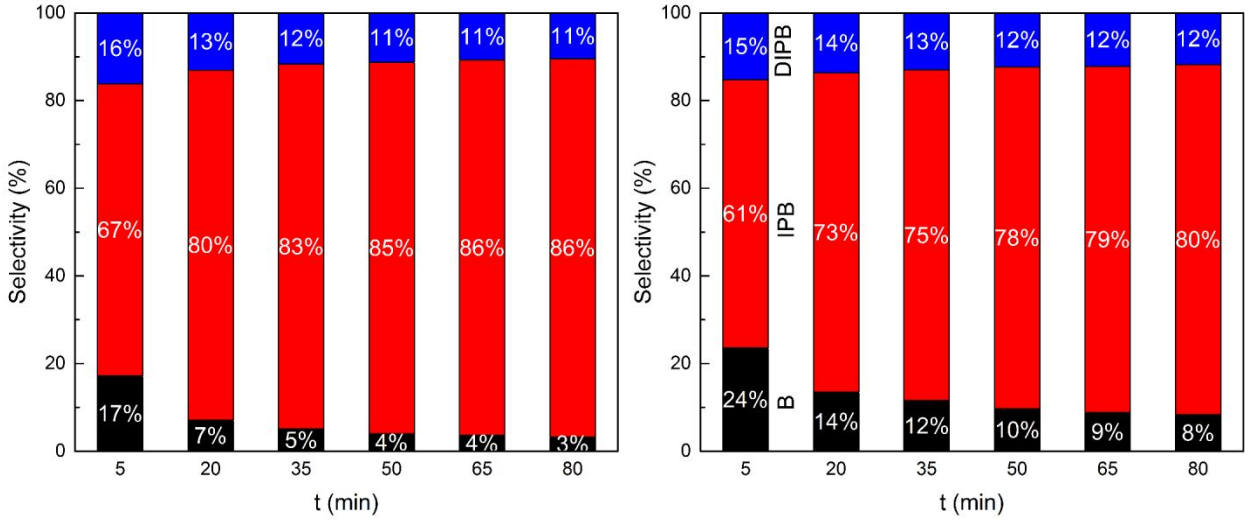

Figure S7. Product selectivity of the USY (left) and [Al,Zr]-USY (right) zeolites (B: benzene, IPB: isopropylbenzene, DIPB: Diisopropylbenzene).

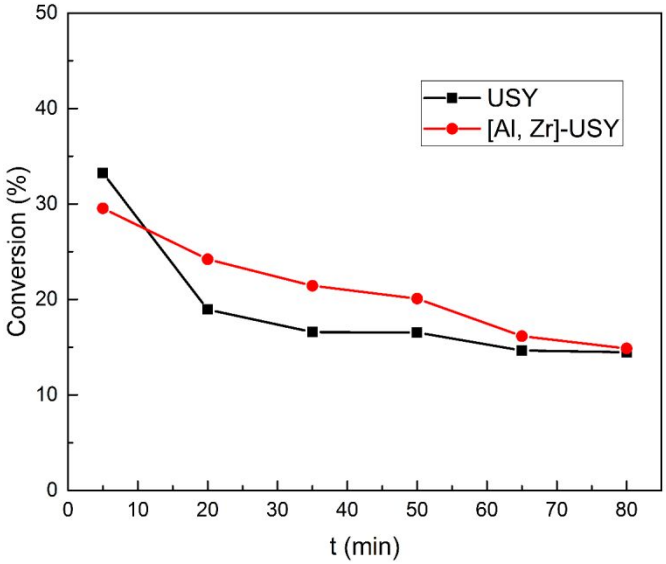

Figure S8. Deactivation of the USY and [Al,Zr]-USY for the catalytic conversion of TIPB at 200 °C.