

Supporting information for

Methanol-to-Olefins Process over Zeolite Catalysts with DDR Topology: Effect of Composition and Structural Defects on Catalytic Performance

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Table S1. Refinement data for Sigma1-315-M.

Crystal system	Trigonal
Space group	<i>R</i> -3 <i>m</i> (№ 166)
<i>a</i> / Å	13.8068(1)
<i>b</i> / Å	13.8068(1)
<i>c</i> / Å	40.8500(1)
$\alpha, \beta, \gamma / ^\circ$	90
<i>V</i> / Å ³	6715.86(1)
<i>Z</i>	12
Wavelength / Å	Co-K α / 1.78897
<i>T</i> / K	293
<i>D</i> _{calc} / g·cm ⁻³	1.783
2 θ range / °	5 – 50
<i>R</i> _p ⁱ	7.79
<i>R</i> _{wp} ⁱⁱ	11.22

$${}^i R_p = \sum_i |y_{i,0} - y_{i,c}| / \sum_i |y_{i,0}|; {}^{ii} R_{wp} = \left[\sum_i w_i (y_{i,0} - y_{i,c})^2 / \sum_i w_i (y_{i,0})^2 \right]^{1/2}$$

Table S2. Carbon based selectivity of products from Methanol conversion over Sigma-1 zeolites at 450°C.

Sample	Light paraffins (%) ^a	Ethylene (%) ^a	Propylene (%) ^a	Butenes (%) ^a	Coke (%) ^b
Sigma1-120-M	3	25	37	9	26
Sigma1-315-L	2	24	35	10	26
Sigma1-315-M	2	36	35	9	18
Sigma1-315-S	4	39	35	8	14
Sigma1-315-S-m	3	42	41	6	8

^a Integral selectivities calculated for the active period of catalyst (*X* > 98%).

^b Calculated from TGA, assuming that all coke was formed during the active period (*X* > 98%).

Figure S1. Pawley fitting plot of Sigma1-315-M. Pawley fit for Sigma1-315-M. The experimental data are presented as black solid line, calculated one by red dots and difference between them as blue solid line. The Bragg positions of the peaks are represented as green sticks. The blue line represents the difference between experimental data and fitting.

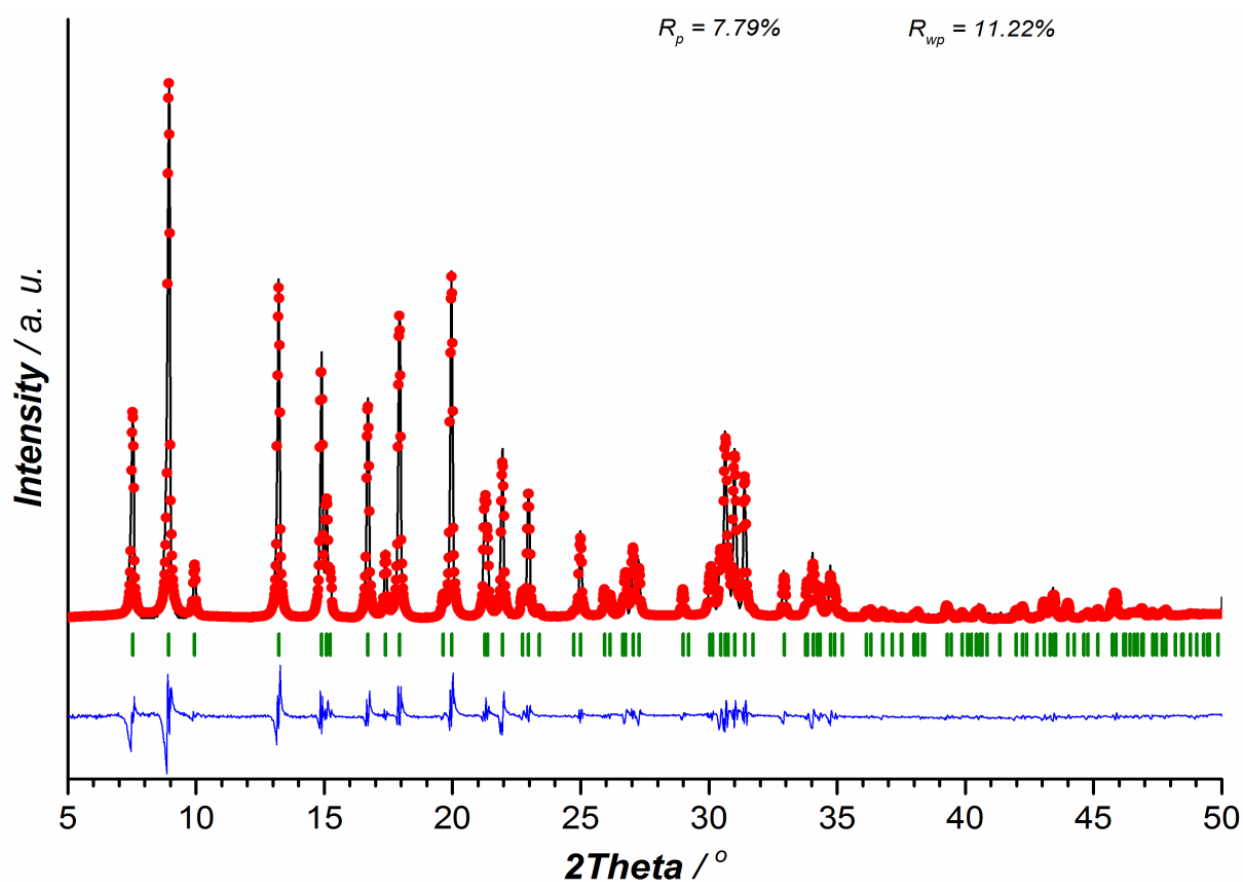


Figure S2. DRIFT spectra of (a) Sigma1-315-S spent at different temperatures; (b) Sigma-1 zeolites with different acidity and crystal size spent at 450 °C.

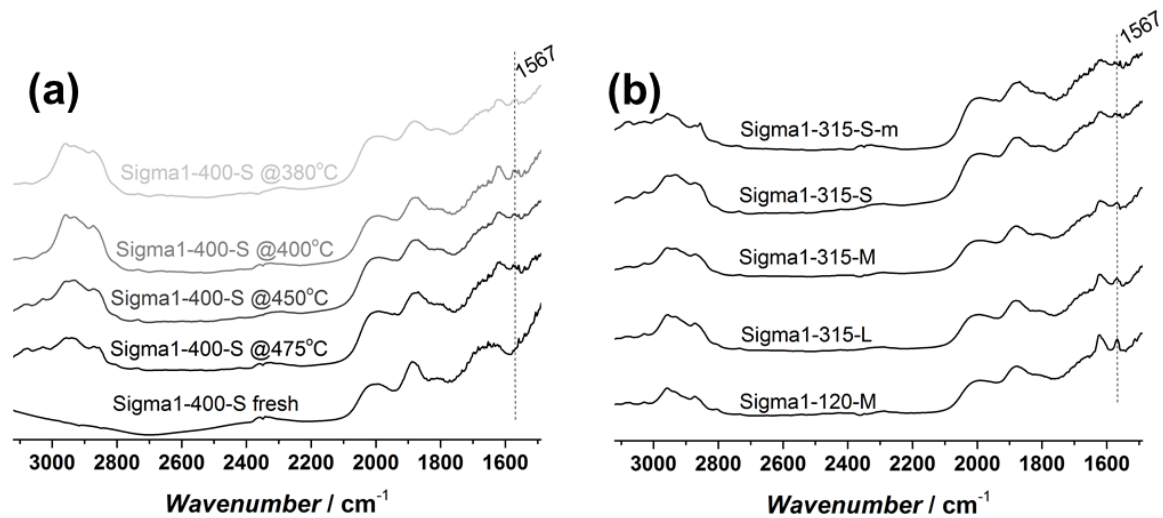


Figure S3. Amount of coke formed in catalysts deactivated at 450 °C as a function of MeOH throughput before deactivation.

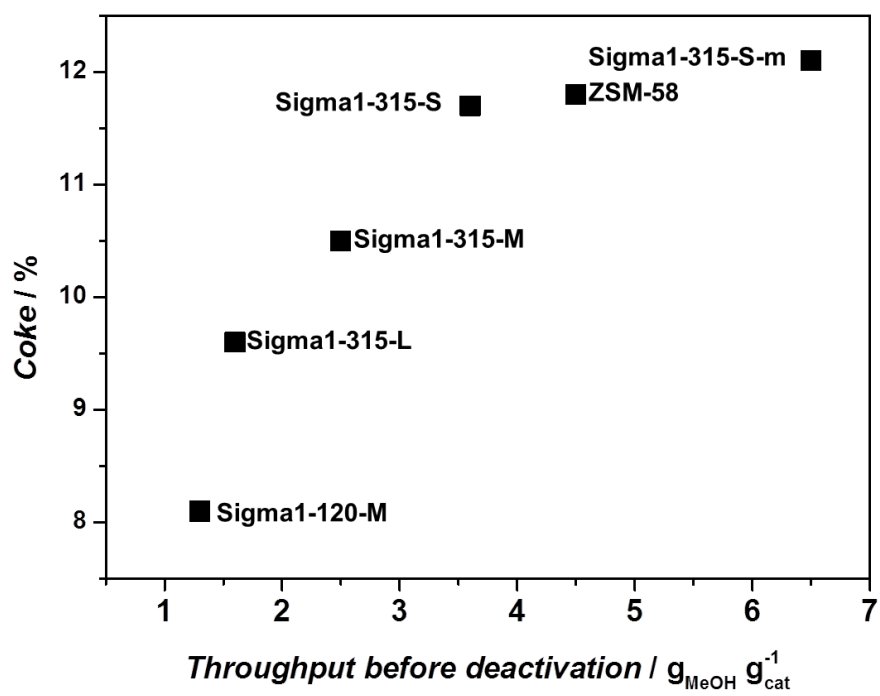


Figure S4. NH_3 TPD profiles of zeolites Sigma1-120-M ($\text{SiO}_2/\text{Al}_2\text{O}_3 = 120$) and ZSM-58 ($\text{SiO}_2/\text{Al}_2\text{O}_3 = 110$).

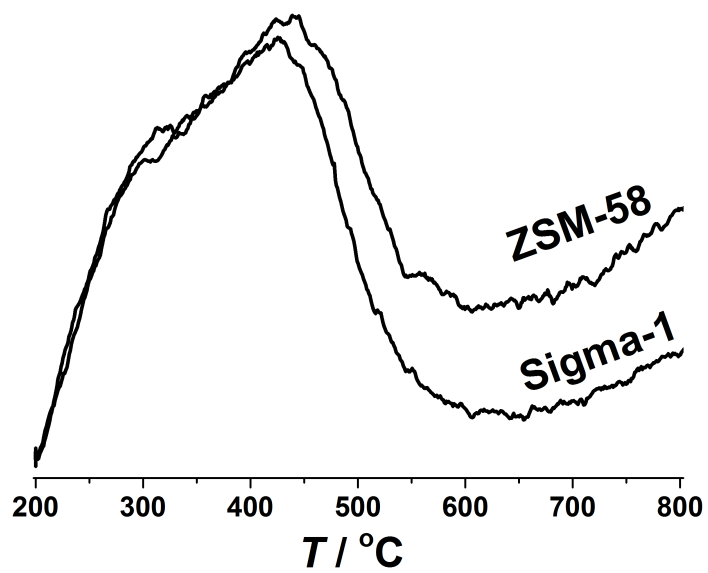


Figure S5. N₂ adsorption-desorption isotherm @ 77 K of Sigma1-315-S and Sigma1-315-S-m catalysts.

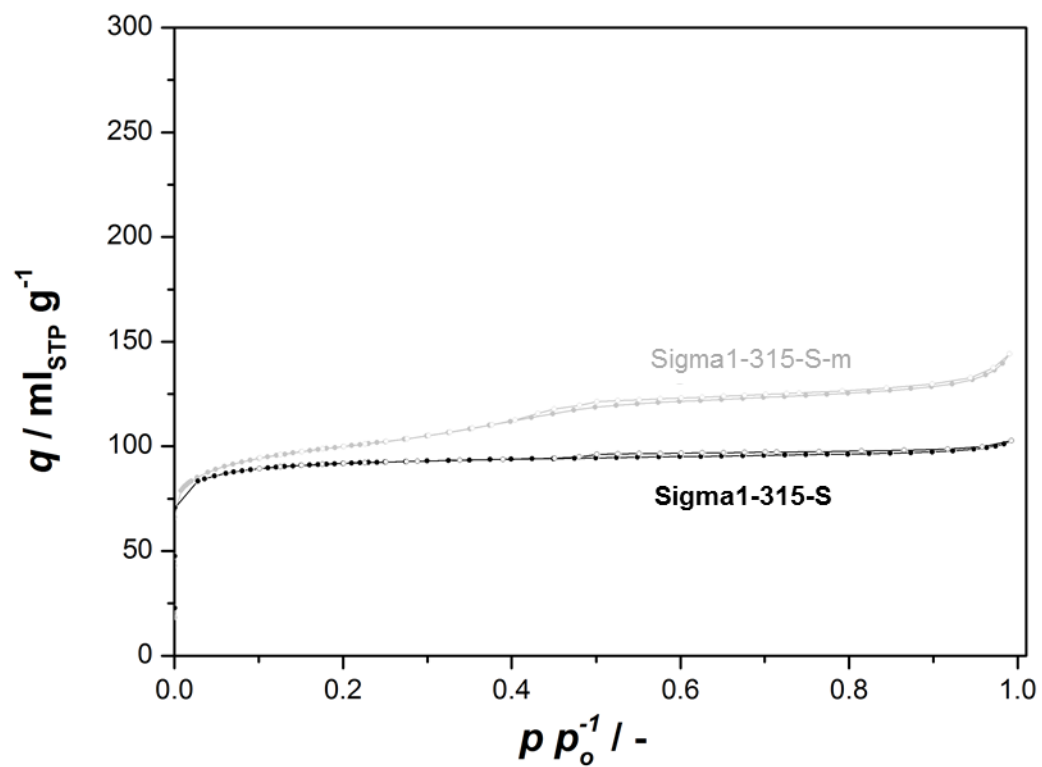


Figure S6. XRD patterns of calcined Sigma1-315-S and Sigma1-315-S-m zeolites.

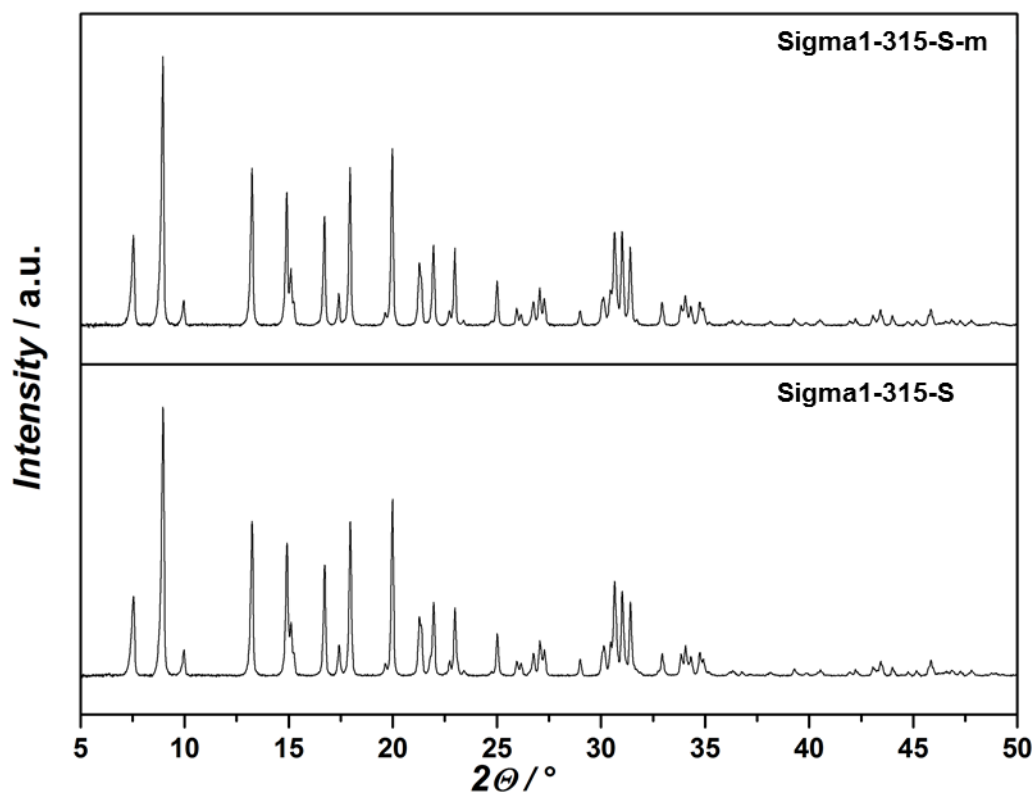


Figure S7. SEM micrograph of ZSM-58 with $\text{SiO}_2/\text{Al}_2\text{O}_3 = 110$.

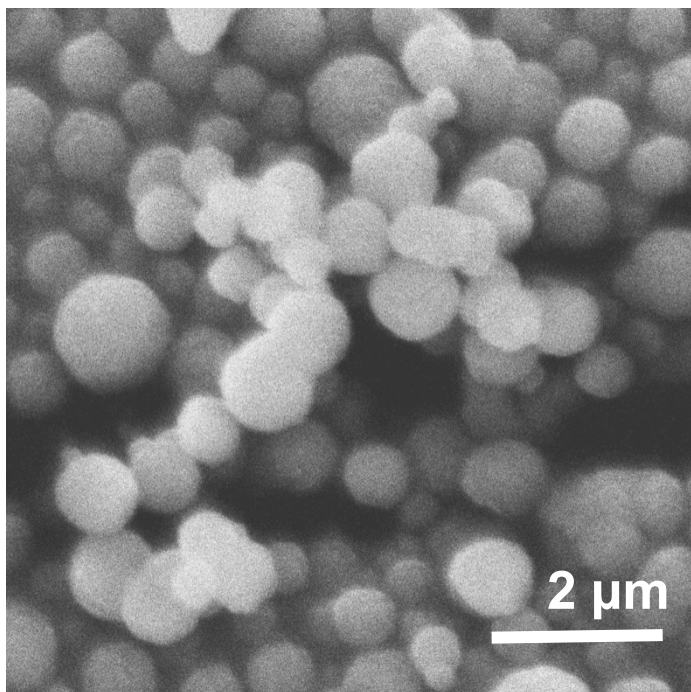


Figure S8. TCD (left) and FID (right) chromatograms showing typical product distribution of MTO reaction performed over zeolites with DDR topology.

