

Ethane and Ethylene Aromatization on Zinc-Containing Zeolites

*Ali Mehdad and Raul F. Lobo**

Center for Catalytic Science and Technology, Department of Chemical and Biomolecular Engineering,
University of Delaware, 150 Academy St., Newark, DE 19716, USA

*Author to whom correspondence should be addressed: lobo@udel.edu

Supporting information

Table S1: Metal content and textural properties of Zn-ZSM-5 with different Si/Al

Si/Al	Zn concentration (M)*	Preparation method	Al (wt%)	Zn (wt%)	Zn/Al (mol/mol)	Micropore volume (cm ³ /g)
11.5	0.0050	IE	3.23	2.18	0.27	0.146
15	0.0050	IE	2.27	0.99	0.18	0.164
25	0.0050	IE	1.42	0.57	0.17	0.151

*Zn was loaded by IE of 0.005 M of Zn(NO₃)₂·6H₂O at T=343 K.

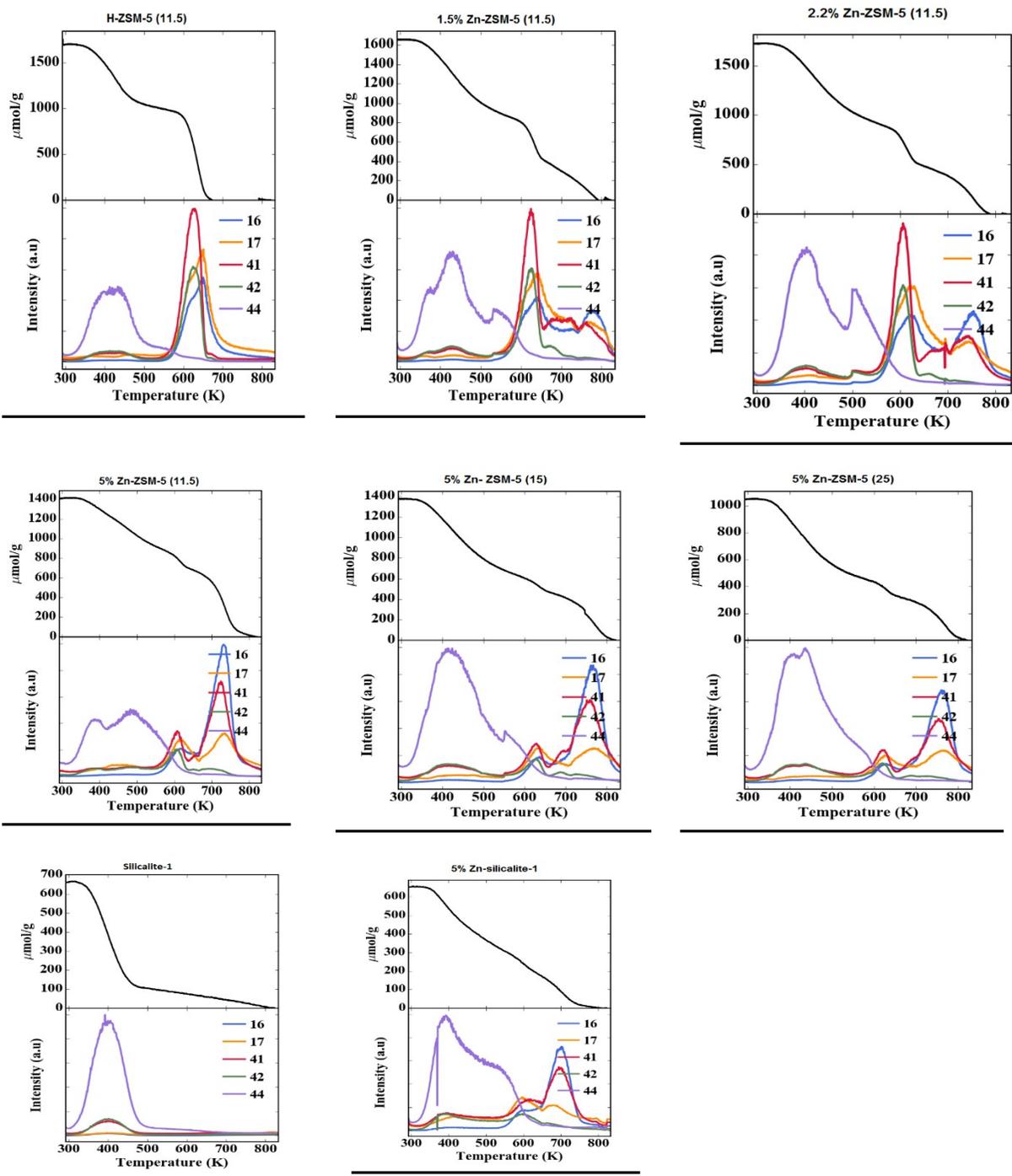


Figure S1: TPD-TGA of 2-propanamine for different samples.

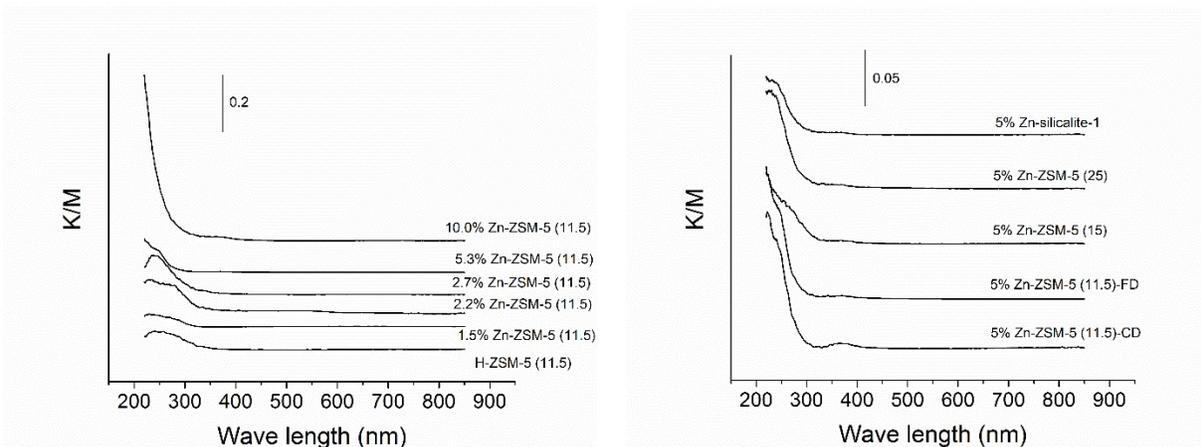


Figure S2: UV-vis diffuse-reflectance spectra of zeolite catalysts as a function of zinc concentration.

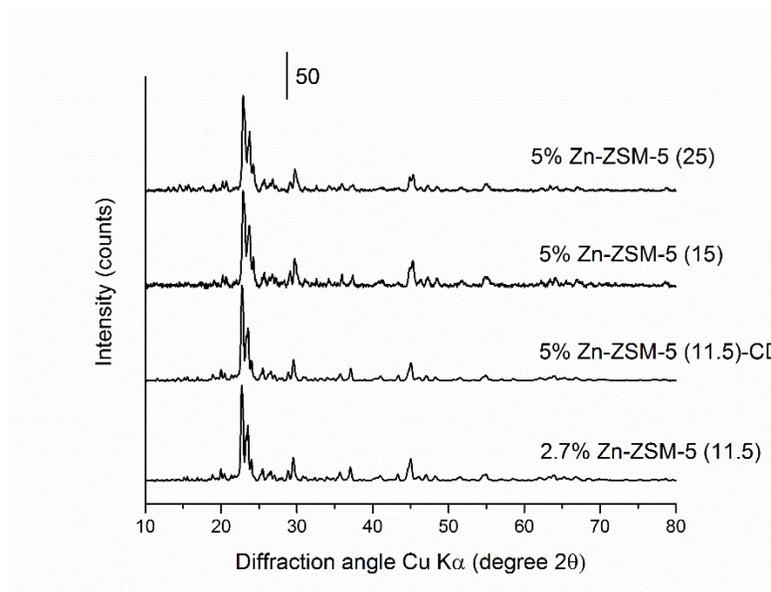


Figure S3: Powder XRD patterns for ZSM-5 with different Zn loading and different Si/Al.

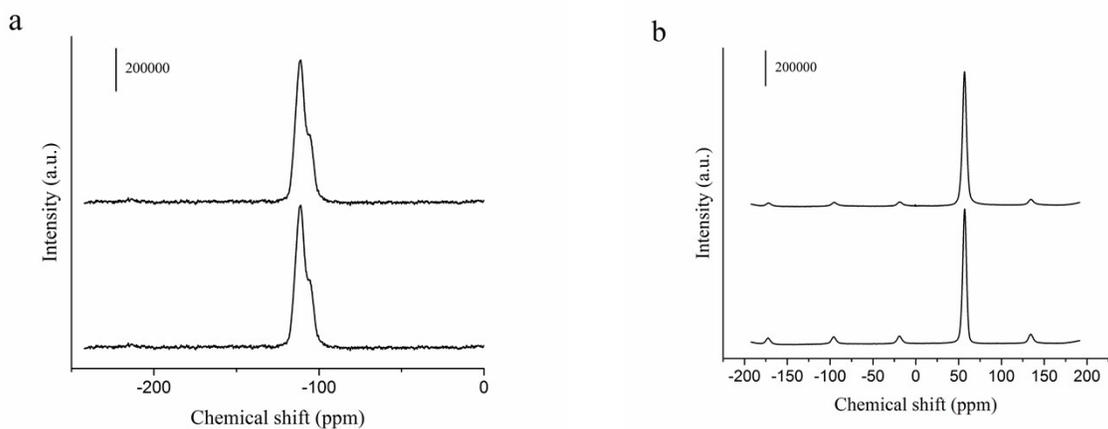


Figure S4: (a) ^{29}Si MAS-NMR and (b) ^{27}Al MAS-NMR for 5% Zn-ZSM-5 (top) and NH₄-ZSM-5 (bottom).

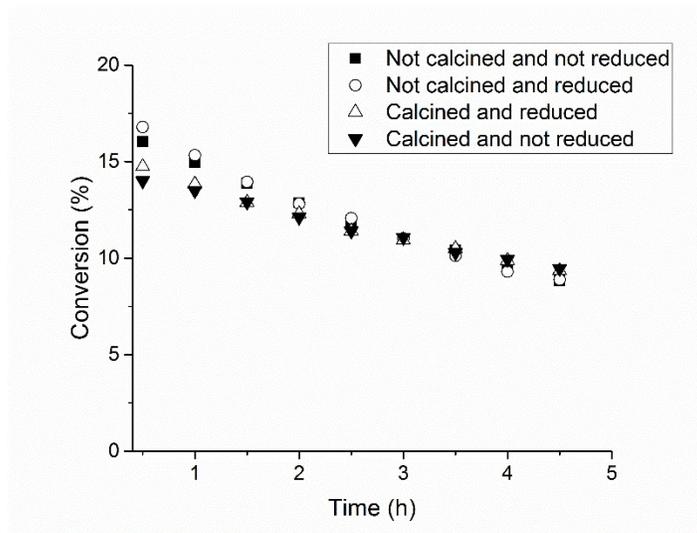


Figure S5: Effect of catalyst pretreatment on ethane conversion over 2.7% Zn-ZSM-5 (11.5). Reaction conditions: 16.5% ethane/He, WHSV= 0.12 g.(g_{cat}.min)⁻¹, T=773 K, P=1 atm.

Table S2: Initial carbon selectivity ($t=0.5$ h) on 2.7% Zn-ZSM-5 (11.5)
 Reaction conditions: 16.5% C₂H₆/He, WHSV=0.12 g_.(g_{cat.}·min)⁻¹, T=773 K and P=1 atm.

Pretreatment	Conv. (%)	Selectivity (mol%)			
		Methane	Ethylene	Benzene	Toluene
Not calcined- Reduced	16.8	5.2	39.2	26.0	21.5
Not calcined- Not reduced	16.0	4.6	42.2	24.9	20.4
Calcined-reduced	14.8	4.1	43.2	24.3	20.2
Calcined-Not reduced	14.0	3.9	43.1	24.5	20.2

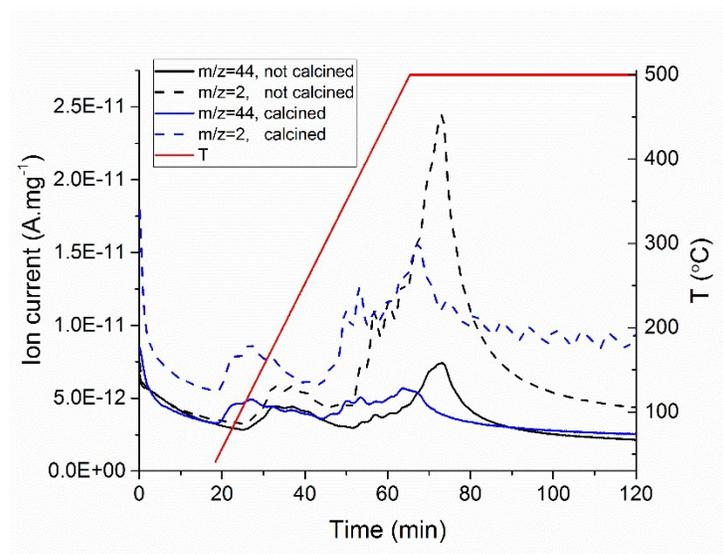


Figure S6: Reduction of 2.2% Zn-ZSM-5 (11.5) in 5% CO/He, and total flow rate of 50 (ml/min).

Table S3: Ethane conversion on Zn-ZSM-5. Reaction conditions: 16.5% C₂H₆/He, WHSV= 0.12 g.(g_{cat} .min)⁻¹, T=773 K and P=1 atm.

Sample*	2.2% Zn-ZSM-5 (11.5)		1% Zn-ZSM-5 (15)		0.6% Zn-ZSM-5 (25)	
Time (h)	0.5	5	0.5	5	0.5	5
Conv. (%)	11.9	9.4	4.2	4.6	2.5	2.6
	Selectivity (mol%)					
Methane	2.0	1.3	0.5	0.6	-	0.4
Propane	1.6	0.7	-	-	-	-
Butane	0.2	0.2	-	-	-	-
Ethylene	55.4	68.0	85.8	80.9	95.5	89.2
Propylene	4.4	4.7	2.7	3.3	1.3	2.1
Butene	1.5	1.9	0.5	1.5	-	-
Benzene	20.0	13.9	8.4	9.0	2.3	5.8
Toluene	14.8	8.8	5.3	4.7	0.8	2.0

*Zn was loaded by IE of 0.005 M of Zn(NO₃)₂·6H₂O at T=343 K.

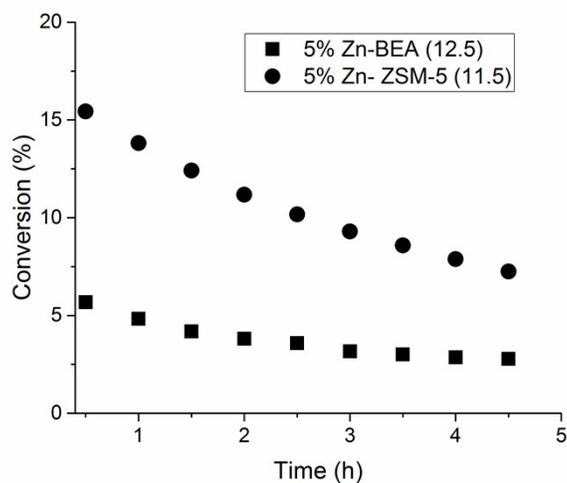


Figure S7: Ethane conversion on 5% Zn-ZSM-5 (11.5) and 5% Zn-BEA (12.5). Reaction conditions: 16.5% C₂H₆/He, WHSV= 0.12 g.(g_{cat} .min)⁻¹, T=773 K and P=1 atm.

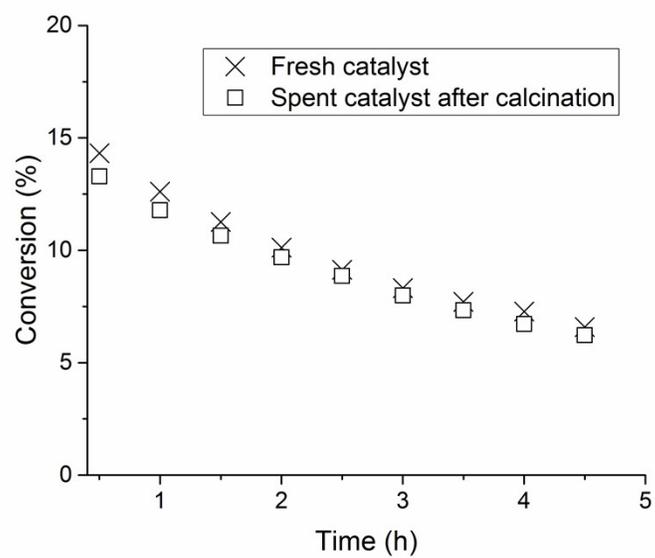


Figure S8: Ethane conversion on fresh and regenerated 5% Zn-ZSM-5 (11.5) catalyst. Reaction conditions: 16.5% C₂H₆/He, WHSV= 0.12 g.(g_{cat} .min)⁻¹, T=773 K and P=1 atm.