

Supplementary Information

Conversion of Ethanol to Butadiene Over Binary MgO-SiO₂ Mixed Oxides Prepared by the
Ammonia Evaporation Method

Ismail Bin Samsudin, Stephan Jaenicke and Gaik-Khuan Chuah,*

Department of Chemistry, National University of Singapore, 3 Science Drive 3, Kent Ridge,
Singapore 117543

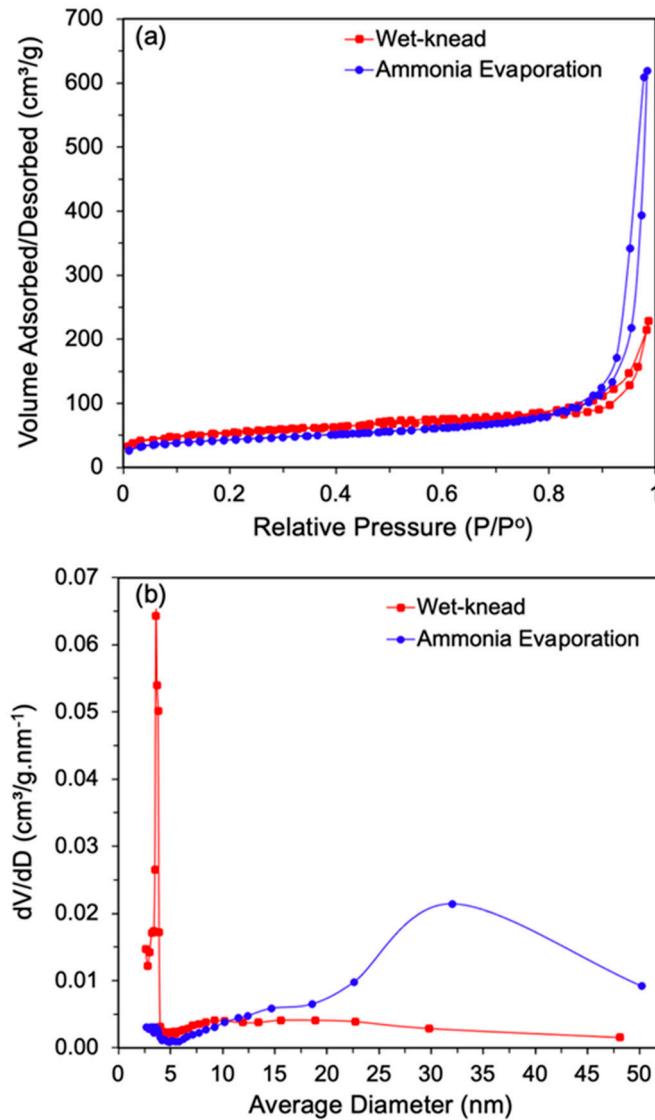


Figure S1. (a) Nitrogen sorption isotherms and (b) pore size distributions of $\text{SiO}_2\text{-MgO-4}$ catalysts prepared by ammonia evaporation and wet-knead methods.

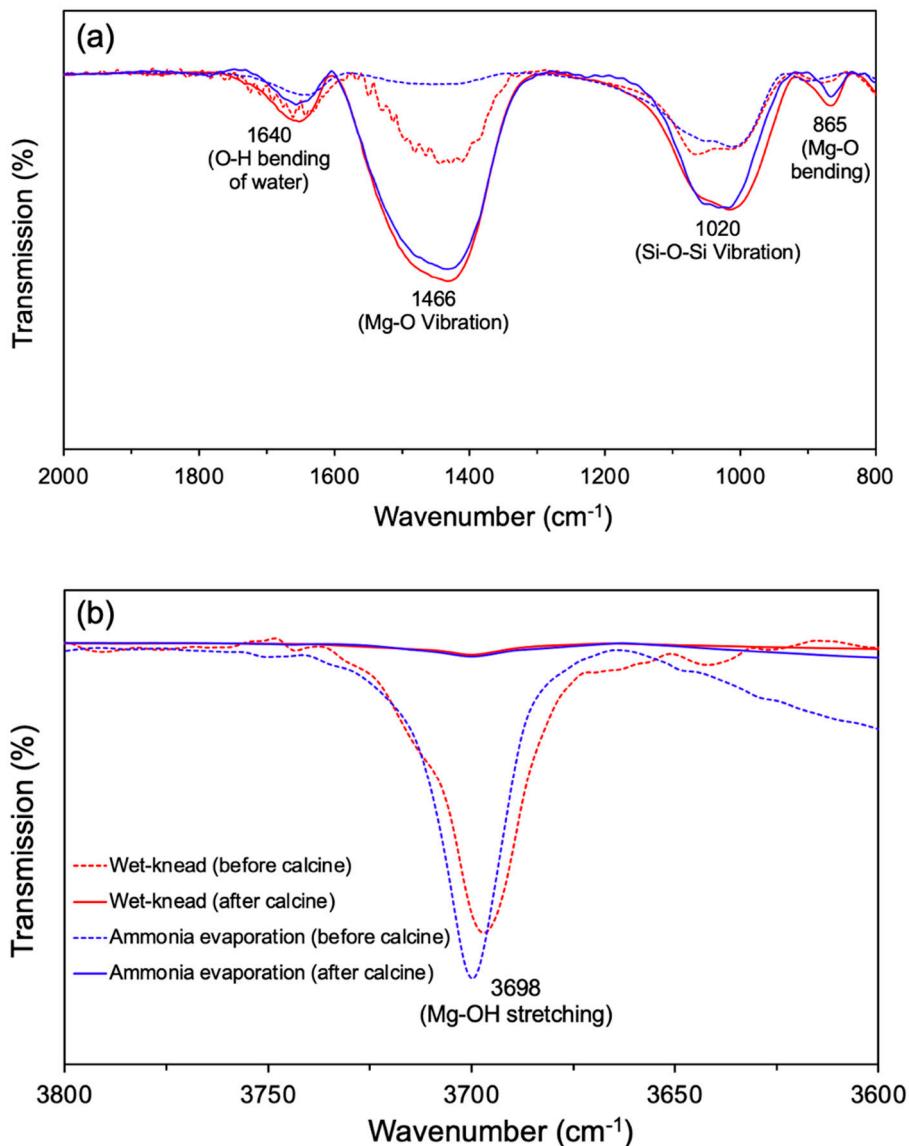


Figure S2. FTIR of MgO-SiO₂ catalysts prepared by ammonia evaporation and wet kneading, before and after calcination at (a) low wavenumbers and (b) high wavenumbers.

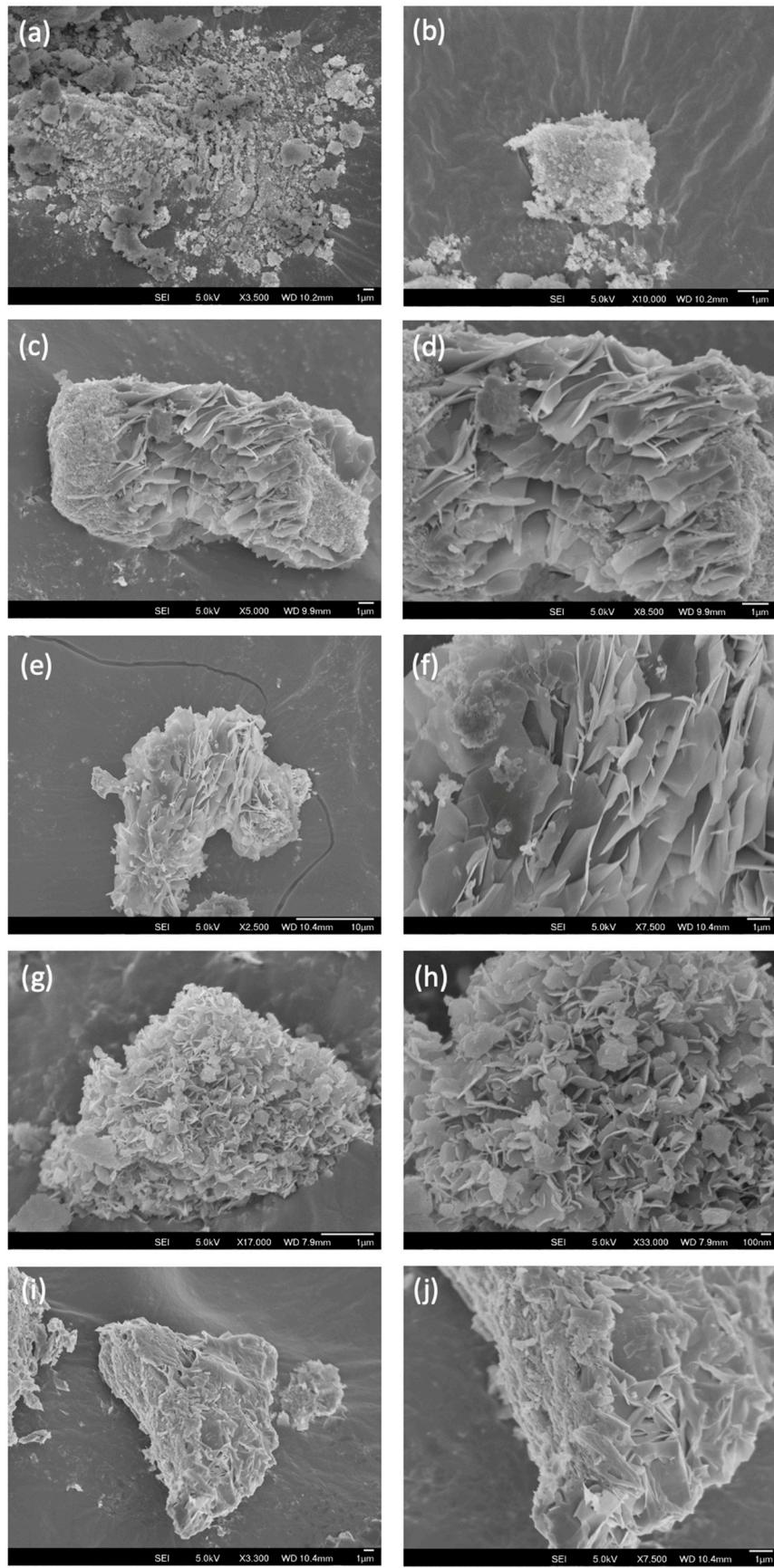


Figure S3. FESEM images of (a, b) SiO_2 and ammonia-evaporated (c, d) $\text{MgO}-\text{SiO}_2$ -0.5, (e, f) $\text{MgO}-\text{SiO}_2$ -1, (g, h) $\text{MgO}-\text{SiO}_2$ -4 and (i, j) $\text{MgO}-\text{SiO}_2$ -10.

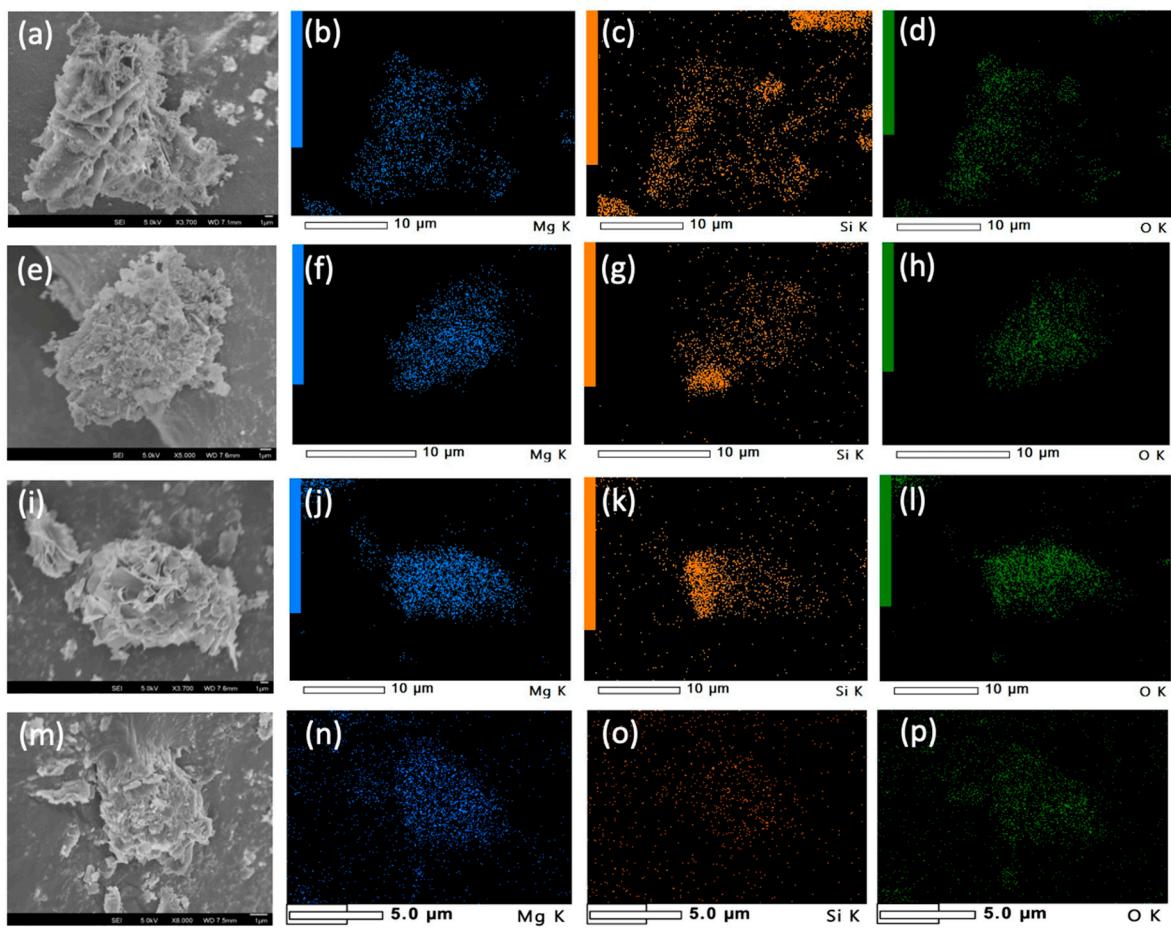


Figure S4. SEM/EDS images of (a-d) MgO-SiO₂-0.5, (e-h) MgO-SiO₂-1, (i-l) MgO-SiO₂-4 and (m-p) MgO-SiO₂-10.

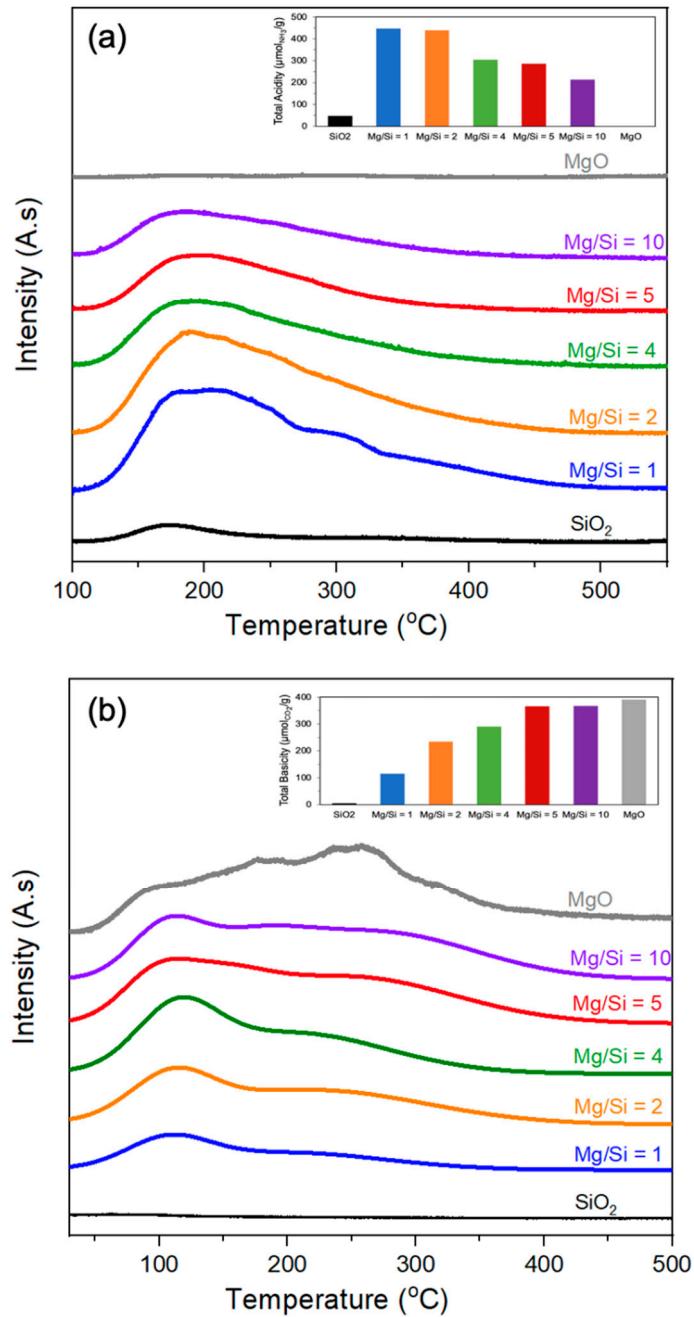


Figure S5. TPD of (a) NH_3 and (b) CO_2 over ammonia-evaporated MgO-SiO_2 catalysts, SiO_2 and MgO . Insert: density of (a) basic and (b) acidic sites.

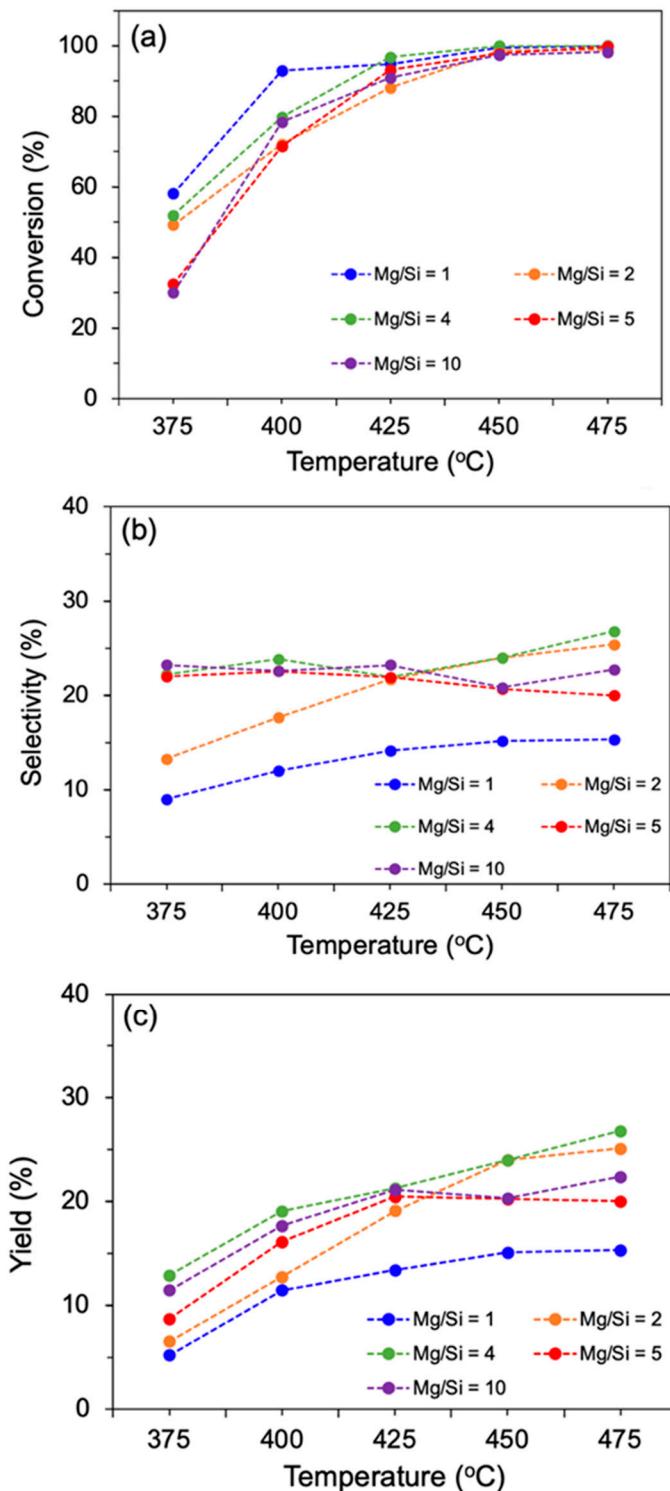


Figure S6. (a) Ethanol conversion (b) BD selectivity and (c) BD yield over MgO-SiO₂ (AE) catalysts at varying Mg/Si ratios and temperatures. Reaction conditions: 0.1 g catalyst, 1.5 g glass beads, 100 µl/h ethanol (3.2 vol% ethanol), 55 ml/min He, TOS = 4 h.

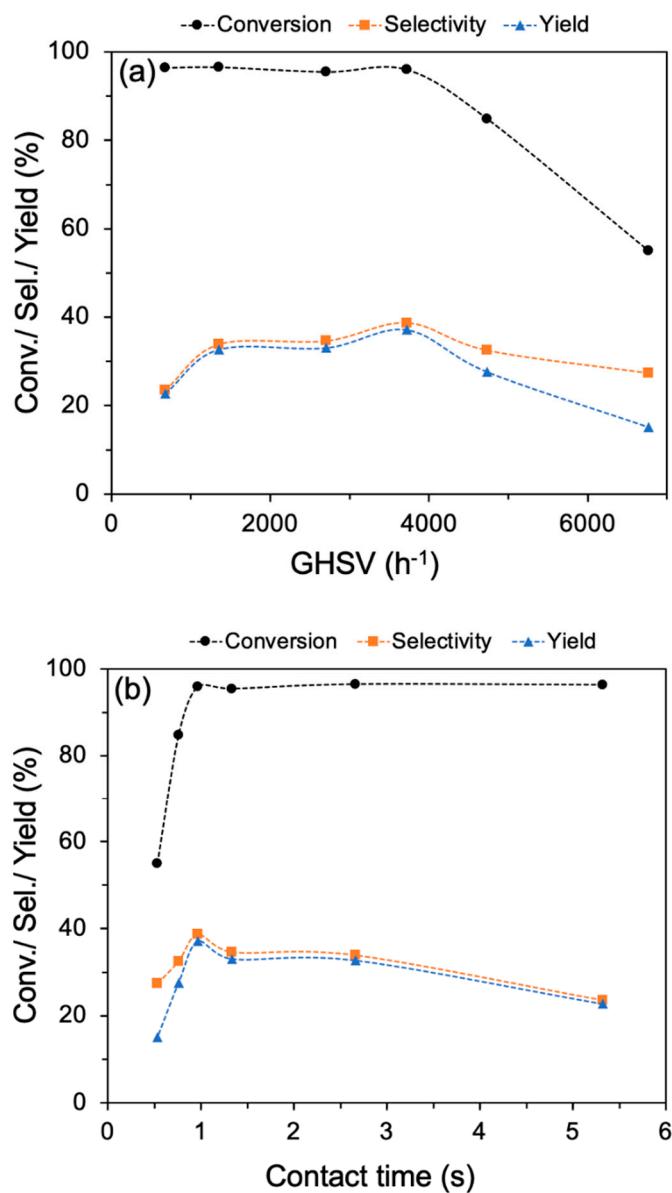


Figure S7. Ethanol conversion, BD selectivity and BD yield over MgO-SiO₂-4 (AE) as a function of (a) GHSV and (b) contact time. Reaction conditions: 0.1 g catalyst, 1.5 g glass beads, 475 °C, 11.3 vol% ethanol.

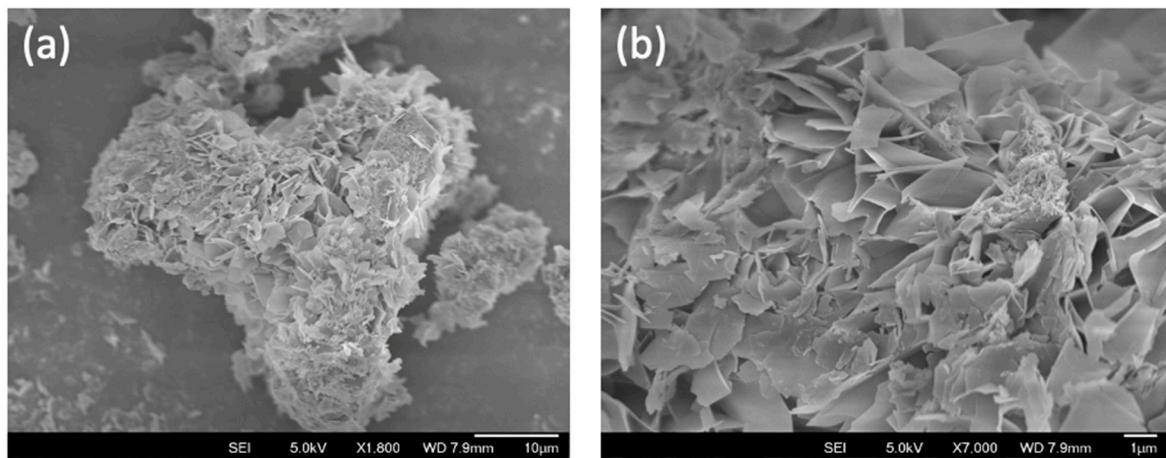


Figure S8. SEM images of MgO-SiO₂-4 (AE) after reaction.

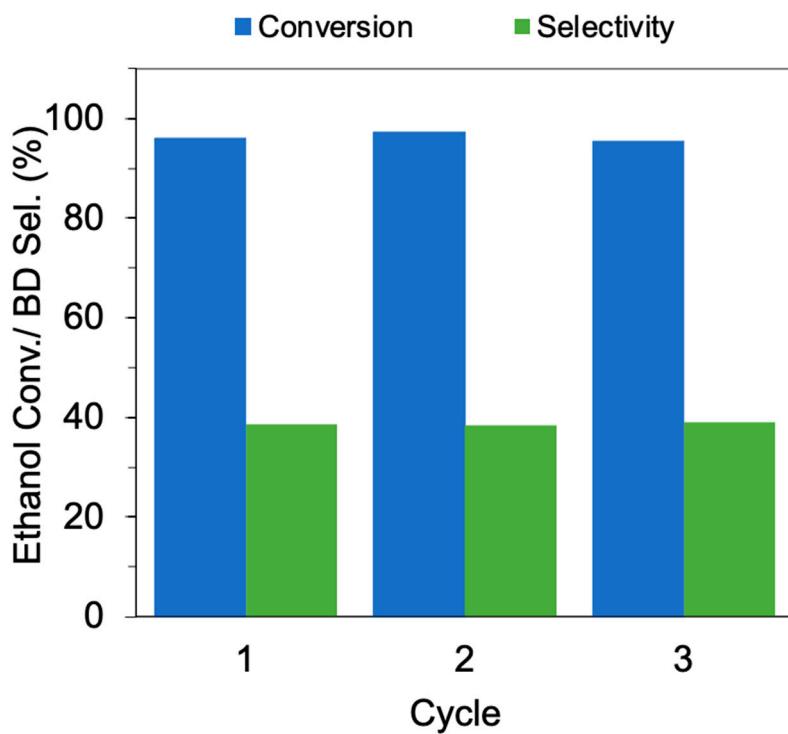


Figure S9. Ethanol conversion and butadiene selectivity over MgO-SiO₂-4. Cycle 1: fresh catalyst, cycles 2 and 3: regenerated catalyst.

Table S1. Density of acidic and basic sites from NH₃ and CO₂ TPD

Sample	Number of acidic sites (μmol NH ₃ /g)	Number of basic sites (μmol CO ₂ /g)
MgO-SiO ₂ -1 (AE)	447	115
MgO-SiO ₂ -2 (AE)	439	235
MgO-SiO ₂ -4 (AE)	305	290
MgO-SiO ₂ -5 (AE)	286	365
MgO-SiO ₂ -10 (AE)	213	367
MgO-SiO ₂ -4 (WK)	362	291
MgO	1	392
SiO ₂	47	5

Table S2. Density of basic and acidic sites of MgO-SiO₂-4 prepared by wet-kneading and ammonia evaporation.

	Number of acidic sites ($\mu\text{mol NH}_3/\text{g}$)			
	Total	Weak	Moderate	Strong
MgO-SiO ₂ -4 (AE)	305	107 (35 %)	143 (47 %)	55 (18 %)
MgO-SiO ₂ -4 (WK)	362	109 (30 %)	170 (47 %)	83 (23 %)
Sample	Number of basic sites ($\mu\text{mol CO}_2/\text{g}$)			
	Total	Weak	Moderate	Strong
MgO-SiO ₂ -4 (AE)	290	131 (45 %)	87 (30 %)	72 (25 %)
MgO-SiO ₂ -4 (WK)	291	81 (28 %)	93 (32 %)	117 (40 %)