Developing Cu-MOR@SiO_2 Core–Shell Catalyst Microcapsules for Two-Stage Ethanol Direct Synthesis from DME and Syngas

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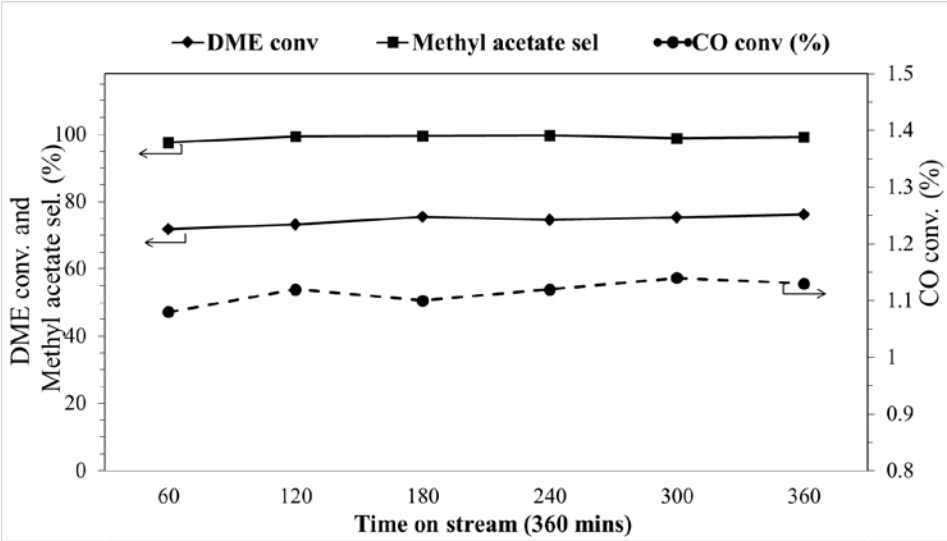

Figure S1. Reaction cond.: pressure = 1.5 MPa, temperature = 220 °C, mass (Cu-MOR@SiO_2) = 0.5 g, gas flow = 45 mL/min, gas mixture: Ar/DME/CO/H_2 = 1.01:2.01:49.50:47.48, TOS = 360 mins.

Single stage DME carbonylation over Cu-MOR@SiO_2 catalyst, Figure S1, was conducted to verify the intermediate product (generated MA) and the influence of side reactions on both catalyst performance and product formation.

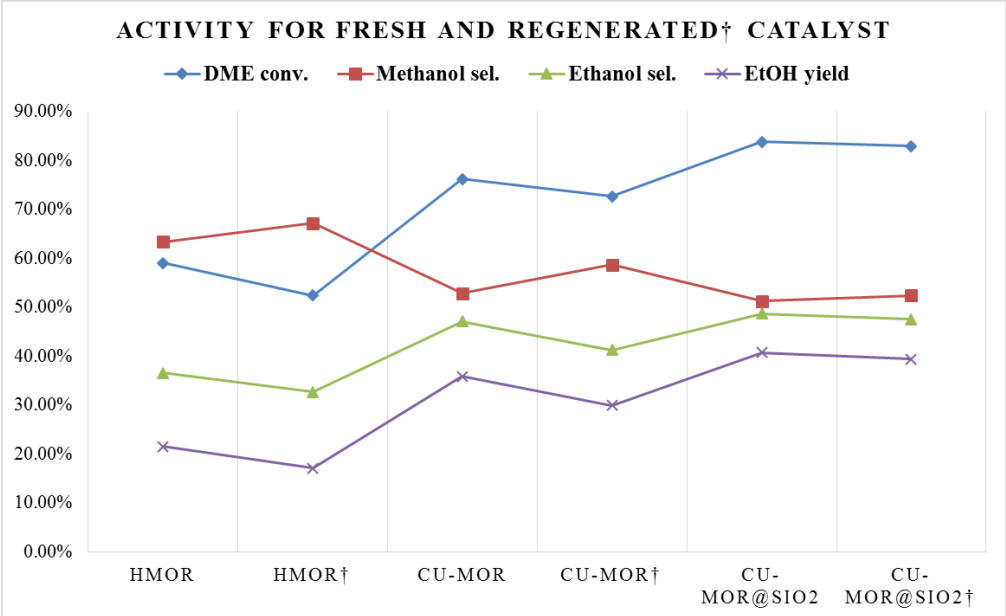

Figure S2. Reaction cond.: pressure = 1.5 MPa, temperature = 220 °C, mass (HMOR/Cu-MOR/Cu-MOR@SiO_2) = 0.5 g, mass (CZA) = 0.5 g, gas flow = 45 mL/min, gas mixture: Ar/DME/CO/H_2 = 1.01:2.01:49.50:47.48, TOS = 360 mins, †Regenerated catalyst.

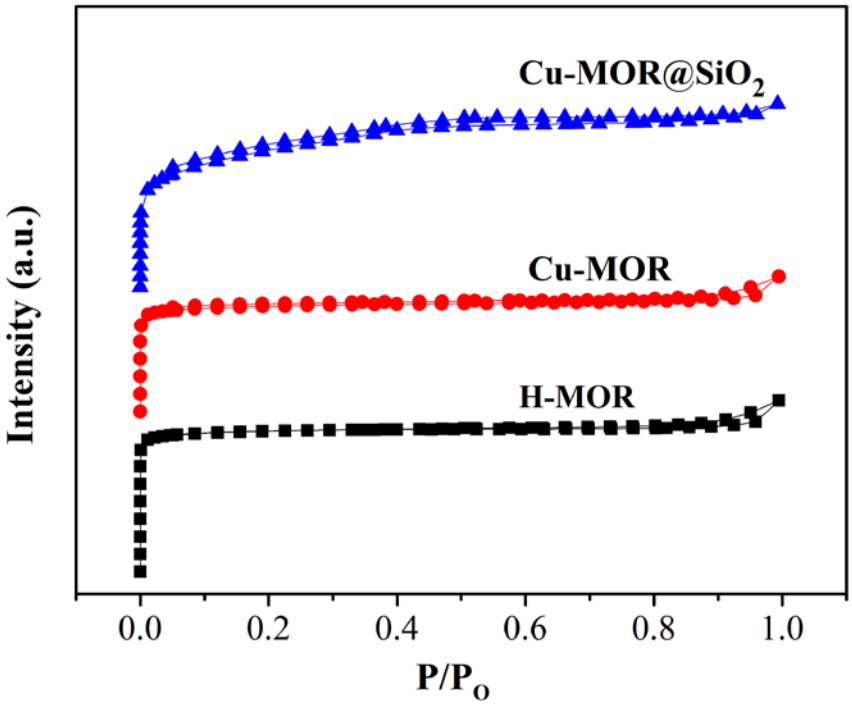

Figure S3. N_2 sorption isotherms for HMOR, Cu-MOR and Cu-MOR@SiO_2 catalysts.

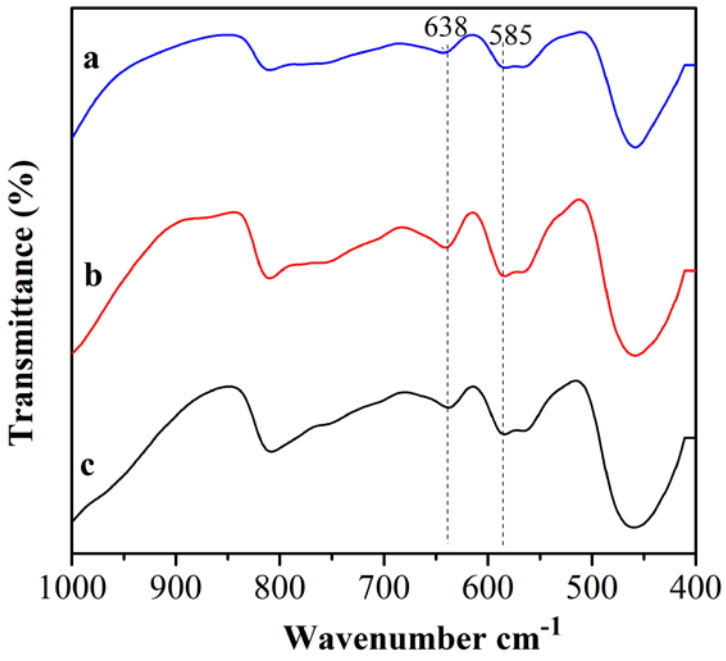

Figure S4. FTIR spectra for **a.** HMOR, **b.** Cu-MOR and **c.** Cu-MOR@SiO_2 catalysts

Figure S5. Images of the as-prepared catalyst samples.

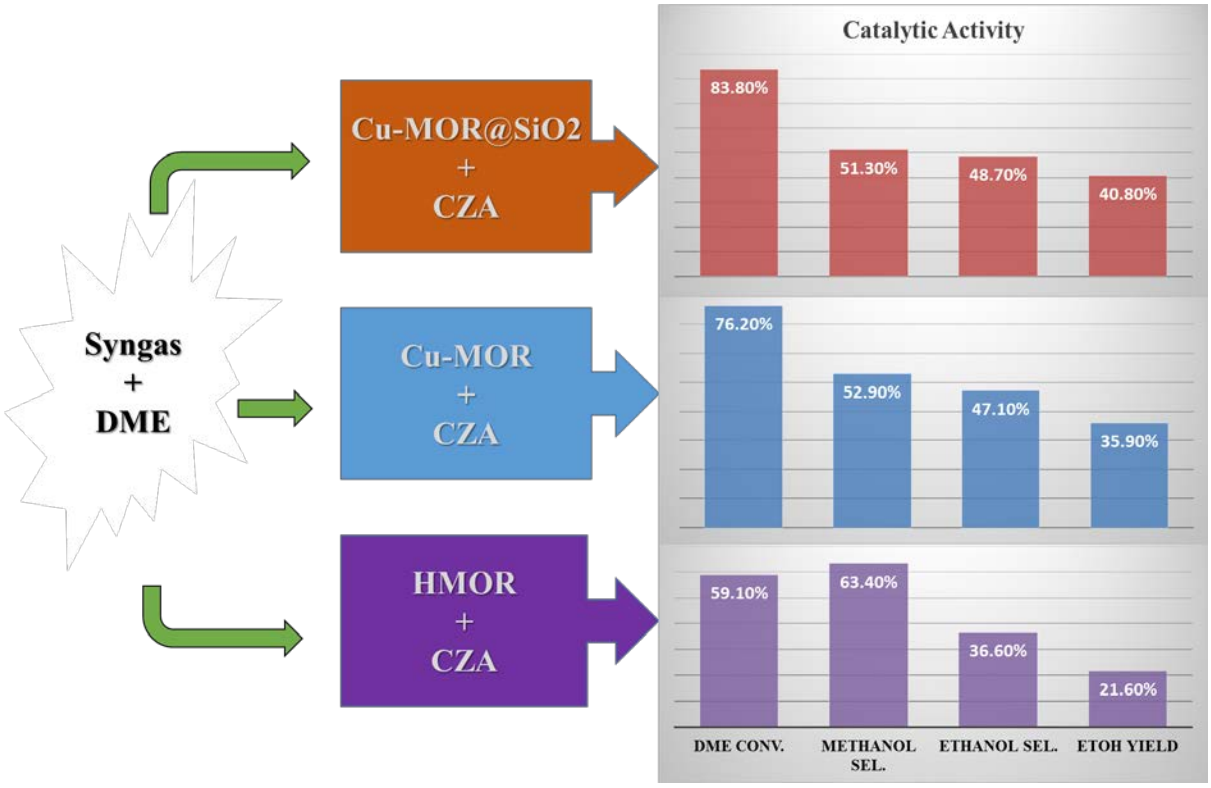

Figure S6. A summary of catalytic activity over the series reactions.

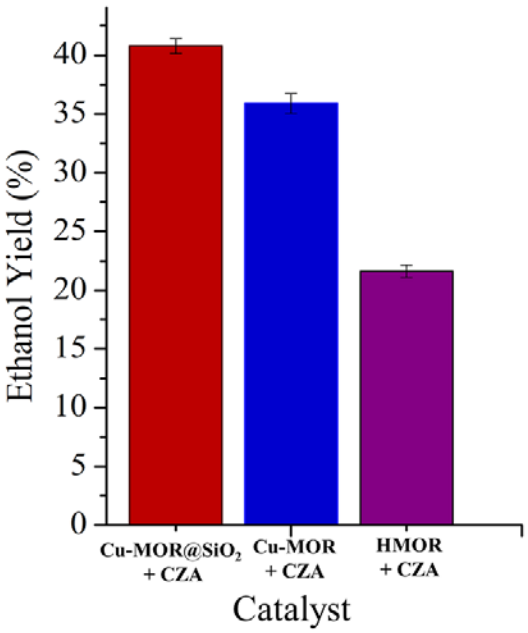

Figure S7. Relative errors represented with error bars.

The experiments for the as-prepared catalysts were conducted for three times, and the results were averaged. The estimated errors are shown in Figure S7 above.

Table S1. BET Surface Area and Total Pore Volume

Catalyst	BET suface area/($m^2 \cdot g^{-1}$)			Pore Volume/($cm^3 \cdot g^{-1}$)		
	Total [a]	Micro[b]	Meso[c]	Total[d]	Meso[e]	Micro[f]
Cu-MOR@SiO_2	405	242	163	0.245	0.121	0.088
Cu-MOR	317	283	34	0.186	0.044	0.147
H-MOR	406	374	32	0.232	0.048	0.194

[a] BET_{total} (Micro[b] + Meso[c])

[b] Micropore (by t-plot)

[c] Mesopore ($S_{Total} = S_{Micro} + S_{Meso}$)

[d] Total pore vol. @ $P/P_0 = 0.95$

[e] Mesopore vol. @ P/P_0=0.95 (BJH method)

[f] Micropore vol. (by t-plot)

H_2-TPR and NH_3-TPD

H_2-TPR was conducted for analyzing the redox behaviour, through hydrogen consumption of the catalyst using a BELCAT-B3 (BEL, Japan) apparatus, furnished with a

thermal conductivity detector (TCD). Prior reduction, the sample (20 mg) was perfectly inserted in a U-tube quartz reactor, then pre-treated under flowing Argon (30 mL· min^{-1}) at 200 °C for 1 h before being cooled to 100 °C. Reduction gas, H_2/Ar (10%, 30 mL· min^{-1}) was fed, at the same time heating from 100 to 650 °C at heat rate of 10 °C min^{-1}.

For NH_3-TPD, the same machine was used but differentiating the parameters. Firstly, the catalyst was purified for 1 h at 200 °C under flowing Helium (30 mL· min^{-1}) then cooled to 100 °C. NH_3 adsorption was carried out at this temperature for 1 h. Helium (30 mL· min^{-1}) was then re-introduced under steady flow to physically desorb NH_3 for another 1 h. The sample was then heated to 650 °C at heat rate of 10 °C min^{-1}. The discharge gas was analyzed online by a thermal conductivity detector (TCD).