Electronic supplementary information (ESI)

Efficient catalytic upgrading of bio-based furfuryl alcohol to ethyl levulinate using mesoporous acidic MIL-101(Cr)

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Catalyst characterization

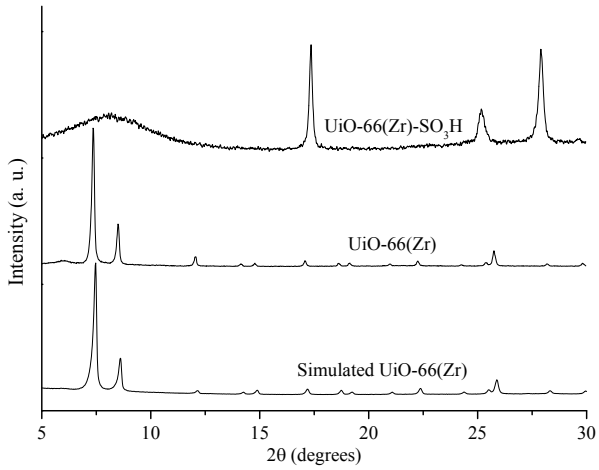


Figure S1 XRD patterns of simulated UiO-66(Zr), UiO-66(Zr) and UiO-66(Zr)-SO_3H

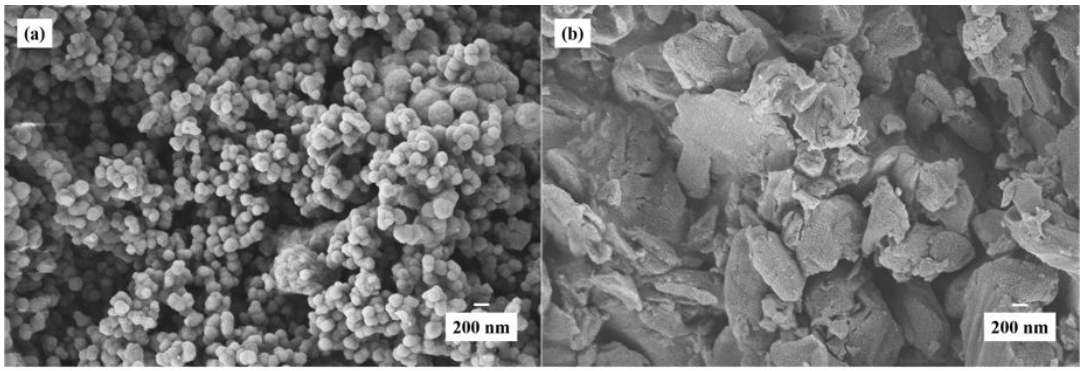


Figure S2 SEM images of UiO-66(Zr) (a) and UiO-66(Zr)-SO_3H (b)

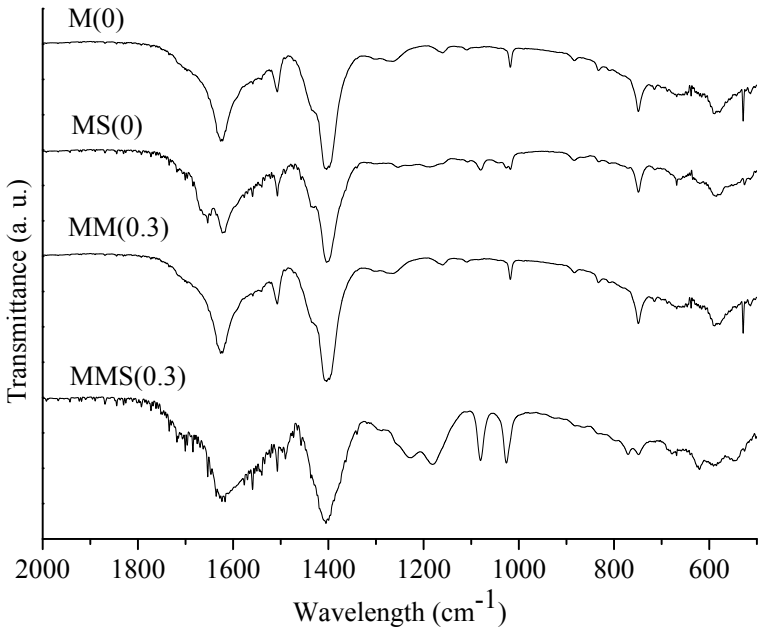


Figure S3 FT-IR spectra of M(0), MM(0.3), MS(0), and MMS(0.3) catalysts

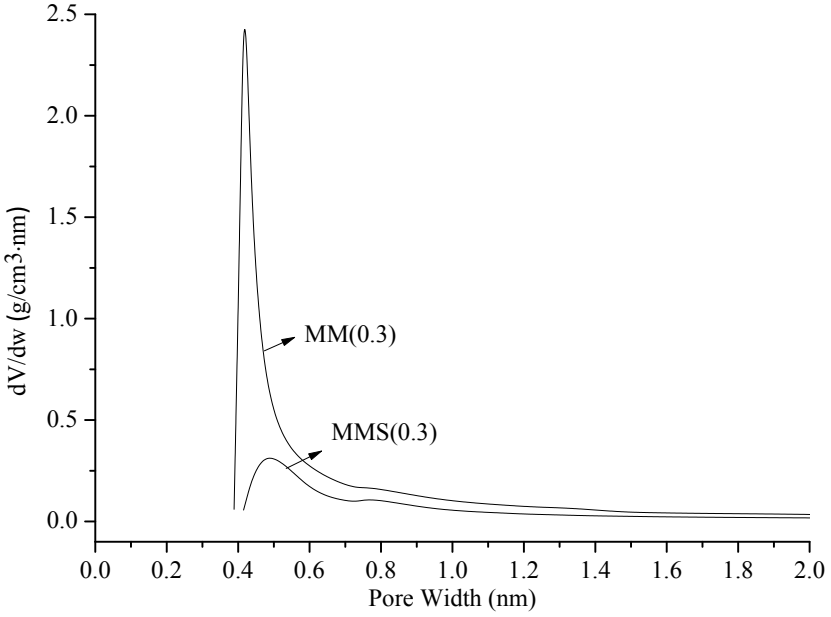


Figure S4 Micropore size distribution of MM(0.3) and MMS(0.3) using Horvath-Kawazoe method

Reaction parameters optimization

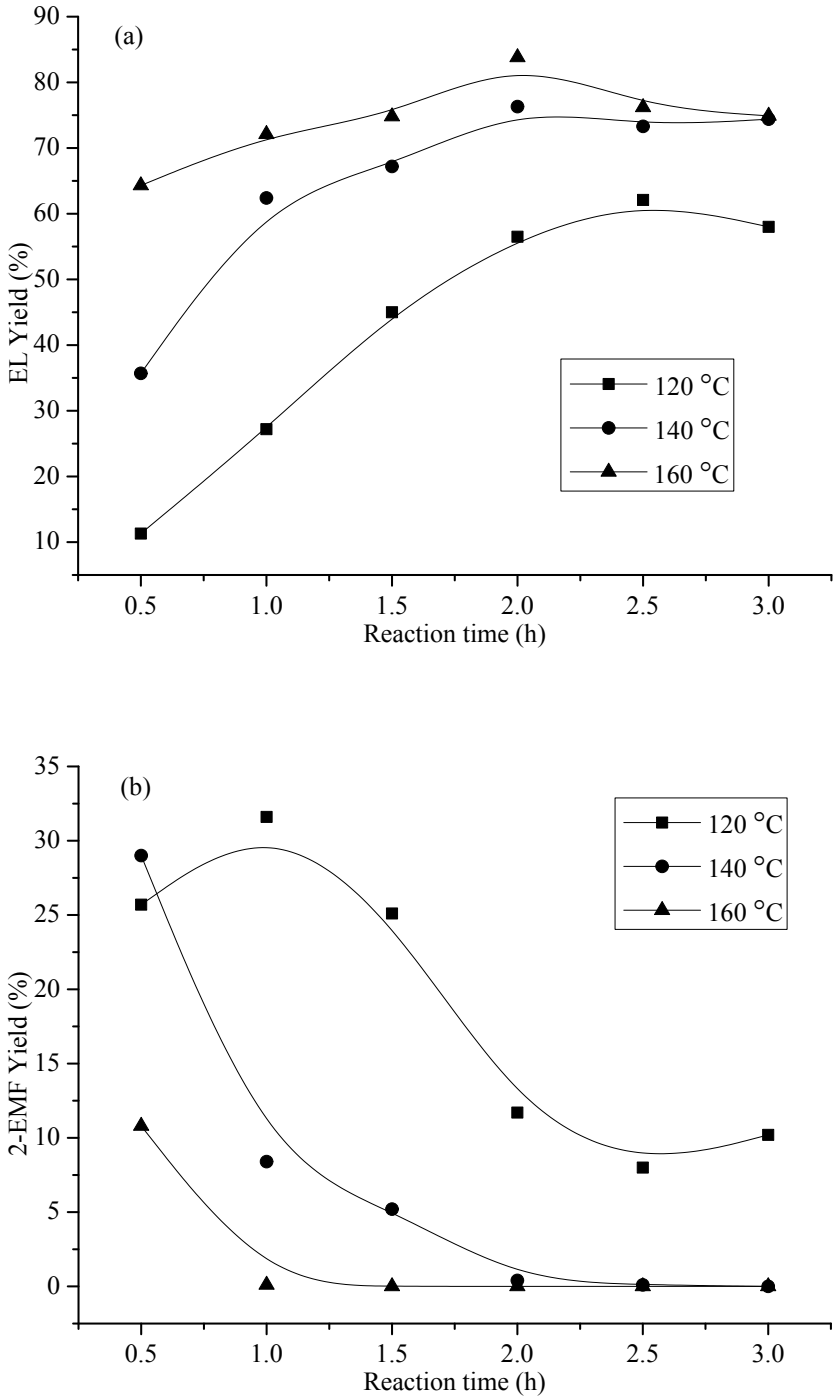


Figure S5 Effects of reaction temperature on catalytic conversion of FA to EL over MMS(0.3)-0.15: (a) yield of EL, (b) yield of 2-EMF. Reaction conditions: molar ratio of FA/EtOH = 1:60, and 50 mg MMS(0.3)-0.15

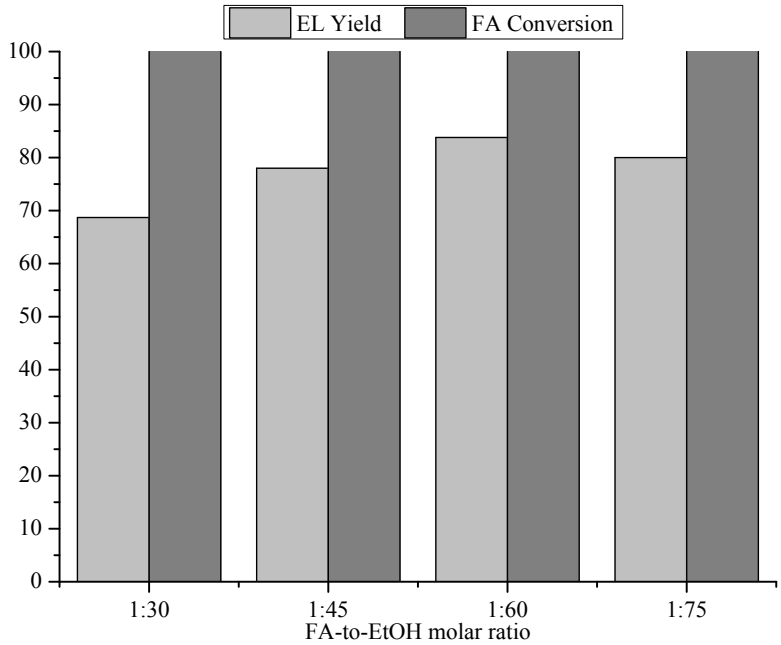


Figure S6 Influence of FA-to-EtOH molar ratio on the catalytic activity of MMS(0.3)-0.15 in ethanolysis of FA to EL. Reaction conditions: 50 mg MMS(0.3)-0.15, 160 ºC, and 2 h

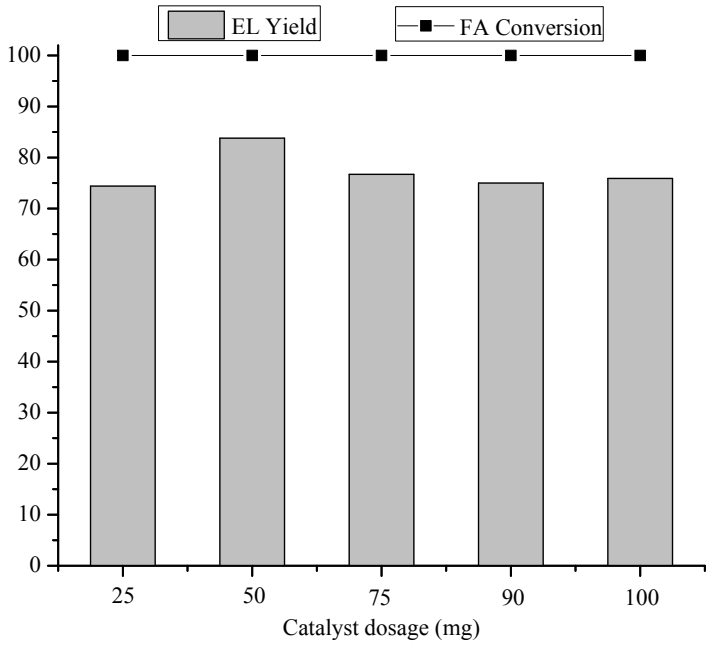


Figure S7 The results of the conversion of FA into EL with different MMS(0.3)-0.15 catalyst amounts. Reaction conditions: molar ratio of FA/EtOH = 1:60, 160 ºC, and 2 h

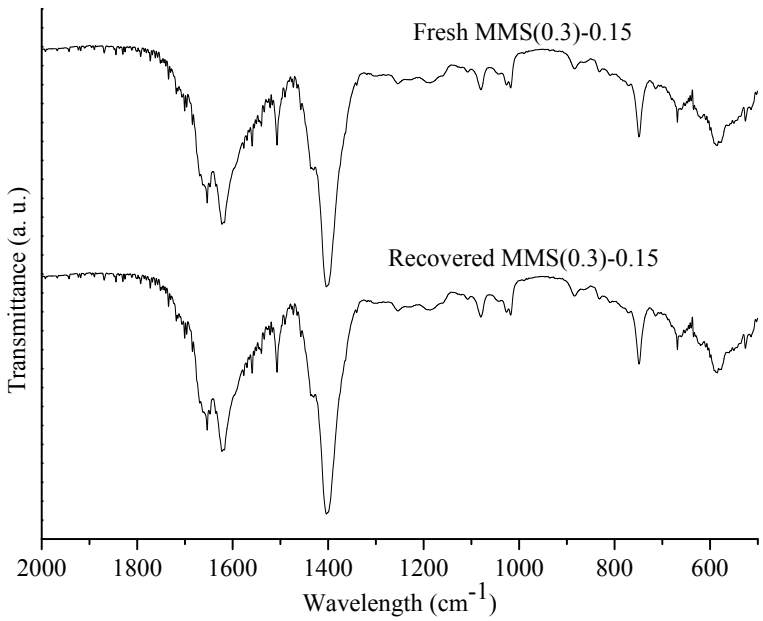


Figure S8 FT-IR spectra of the fresh and recovered MMS(0.3)-0.15 catalysts.

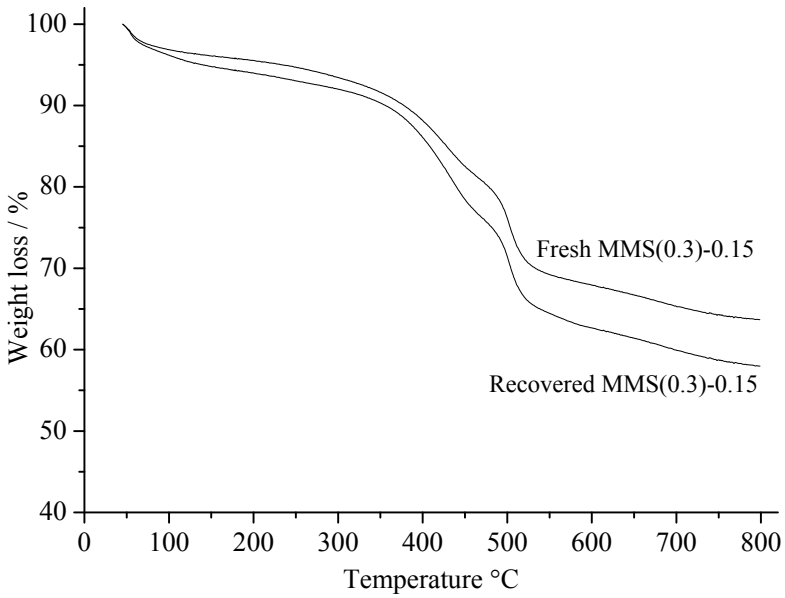


Figure S9 TG curves of the fresh and recovered MMS(0.3)-0.15 catalysts.

Possible mechanism

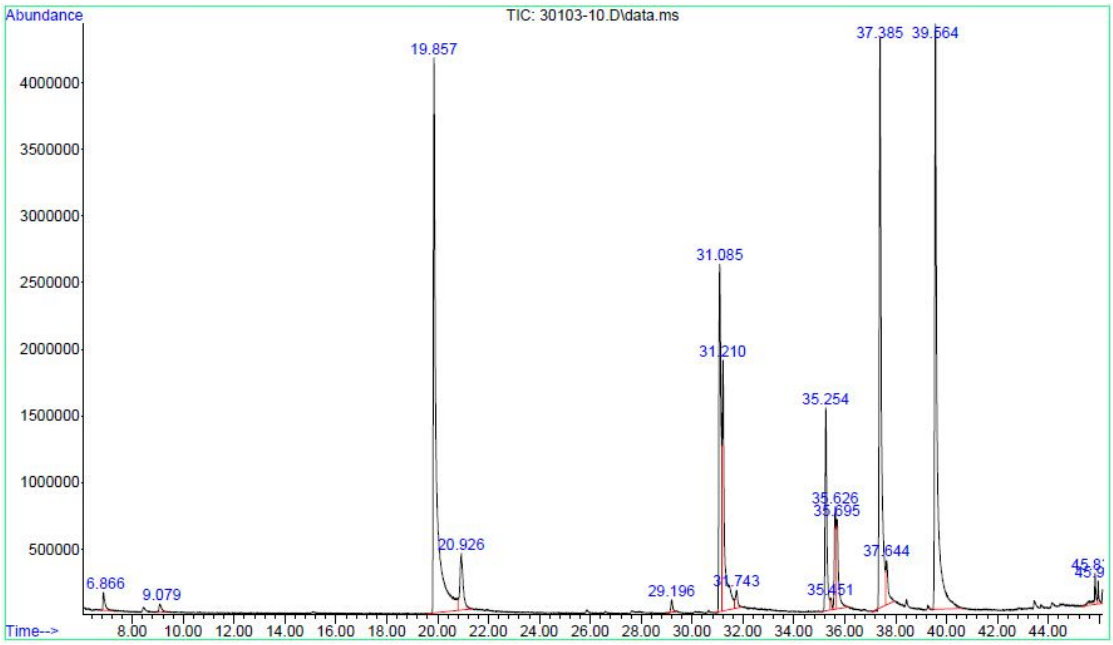


Figure S10 GC-MS spectrum of the intermediates and byproducts formed during the course of the one-pot ethanolysis reaction. Reaction conditions: molar ratio of FA/EtOH = 1:60, 50 mg MMS(0.3)-0.15, 120 ºC, and 1 h

Table S1 The intermediates and byproducts identified by GC-MS during the course of the one-pot ethanolysis reaction. (Reaction conditions: molar ratio of FA/EtOH = 1:60, 50 mg MMS(0.3)-0.15, 120 ºC, and 1 h)

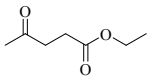
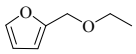
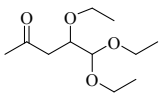
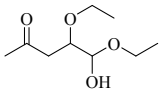
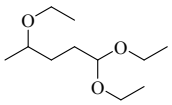
Molecular structure	Name of compound	Retention time	Products
	Ethyl levulinate	31.085	Main product
	2-(Ethoxymethyl)furan (2-EMF)	19.857	Intermediate
	4,5,5-Triethoxypentan-2-one (TEP)	35.626/35.695	Intermediate
	4,5-Diethoxy-5-hydroxypentan-2-one (DHP)	35.254	Intermediate
	2,5,5-Triethoxypentan-2-one	39.564	Byproduct

Table S2 The relative amount of the main product and intermediates at different times identified by GC-MS (Reaction conditions: molar ratio of FA/EtOH = 1:60, 50 mg MMS(0.3)-0.15, 120 ºC)

Time	EL Yield (%)	2-EMF Yield (%)	DHP Yield (%)	TEP Yield (%)
15 min	0.7	6.2	—	—
30 min	11.3	25.7	15.9	7.4
60 min	27.2	31.6	14.7	6.8
120 min	56.5	11.7	3.1	3.7