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Bifunctional Pt-Mo catalyst for in-situ hydrogenation of methyl stearate into alkanes using formic acid as a hydrogen donor

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Preparation of Pt/Mo/AC

Pt/Mo/AC was obtained using the wet impregnation method. Firstly, Mo/AC was prepared by synthesis method of Pt-Mo/AC. Then, appropriate amounts of $\text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}$ were deposited on the Mo/AC support to obtain the precursor $\text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}/\text{Mo}/\text{AC}$, which was loaded in quartz tube and calcined under the same calcination conditions as Pt-Mo/AC.

Gas analysis method

Reactor headspace gas were collected using 0.5 L Restek Tedlar sample bags. The quantitative analysis of CH_4 and H_2 was performed using Shimadzu GC-2014C TCD gas chromatograph outfitted with TDX-01 (3 m×3 mm (ID)) and Porapak Q 60/80 mesh, respectively. CH_4 analysis conditions: N_2 was carrier gas, inlet temperature was 100 °C, an isothermal oven temperature profile was 50 °C. The TCD detector temperature was 200 °C, and the reference gas and auxiliary gas flow were both 20 mL min⁻¹. H_2 analysis conditions: Ar was carrier gas, and the oven temperature was firstly maintained at 30 °C for 3 min, then heated to 150 °C at 20 °C/min for 1 min. The other parameters were the same as the CH_4 analysis conditions.

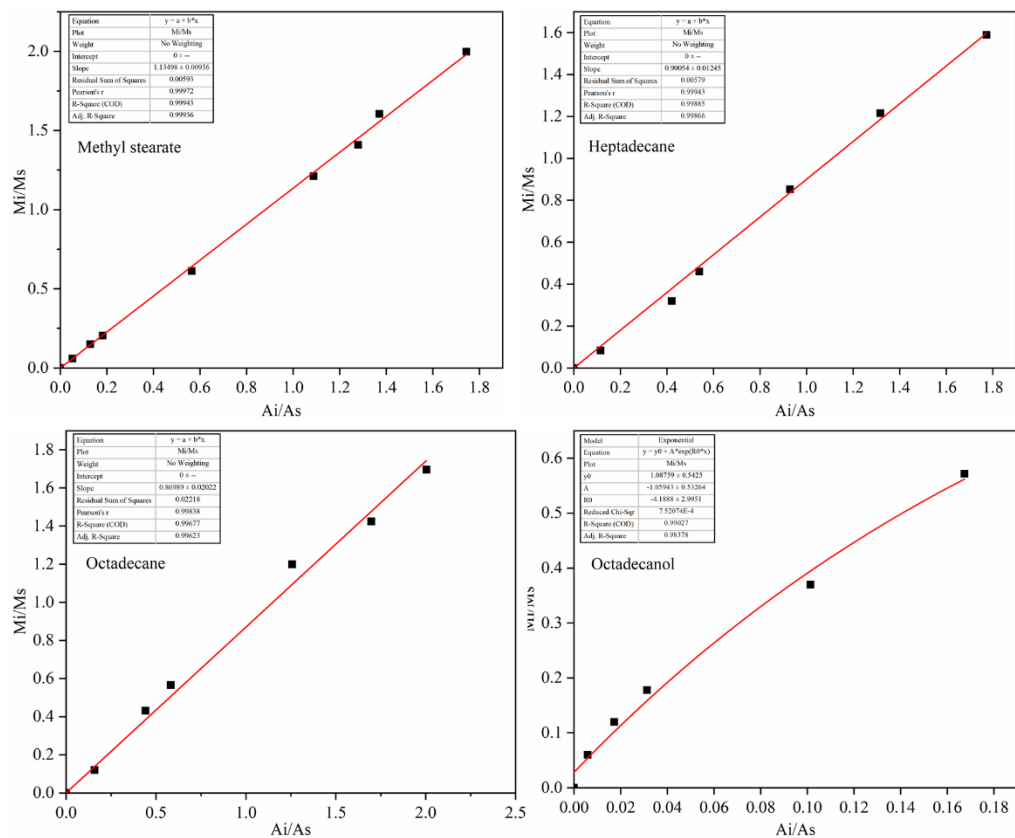


Figure S1. The calibration curves of different substances. M and A refers to mass and area, respectively, and subscript i and s refer to certain substance and internal standard.

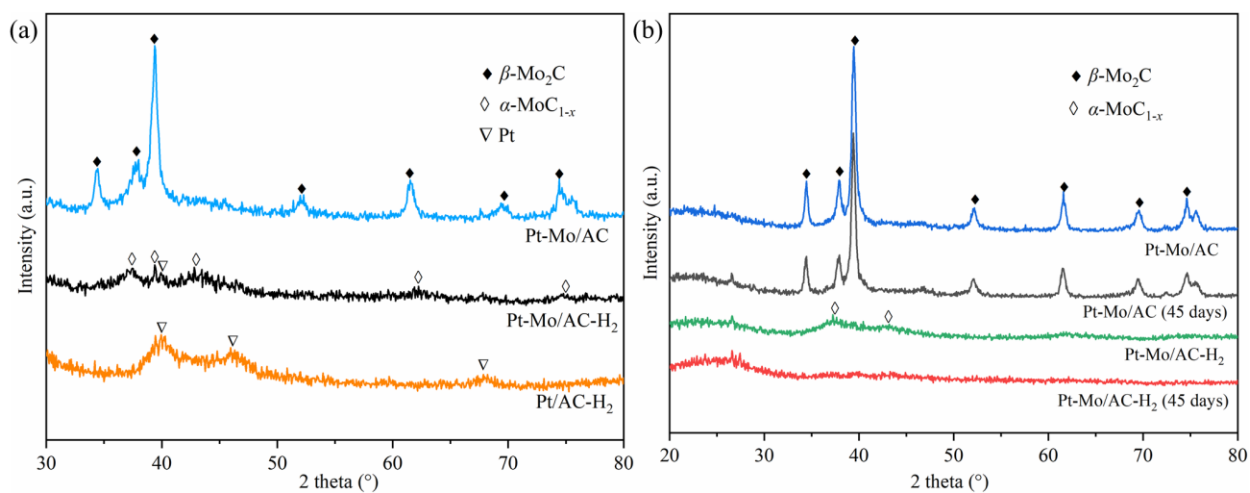


Figure S2. (a) XRD patterns of Pt-Mo/AC, Pt-Mo/AC-H₂ and Pt/AC-H₂ (b) XRD patterns of catalysts. Pt-Mo/AC (45 days) and Pt-Mo/AC-H₂ (45 days) were left in the air for 45 days

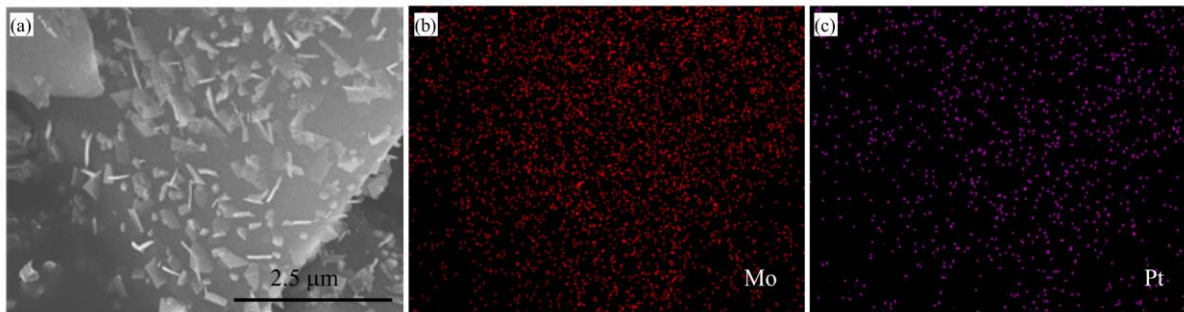


Figure S3. SEM images and EDS mapping of Pt-Mo/AC

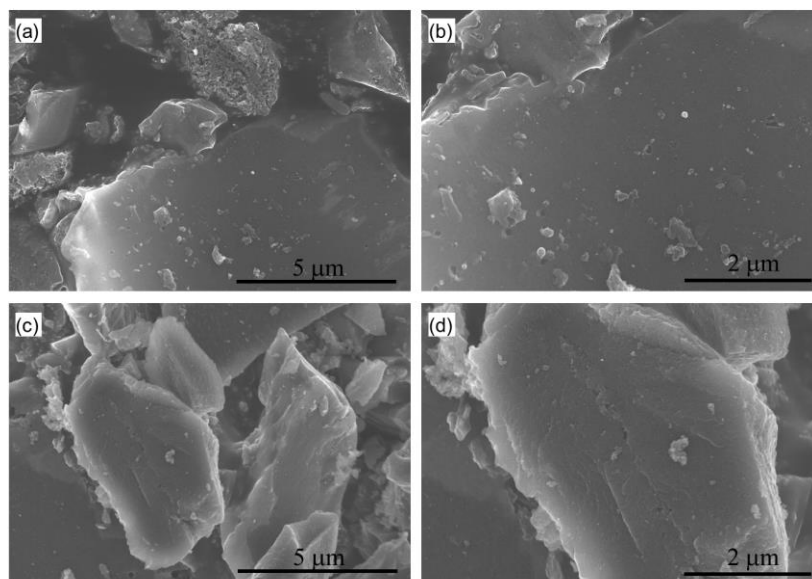


Figure S4. SEM images of Pt-Mo/AC-H₂ (a, b) and AC (c, d)

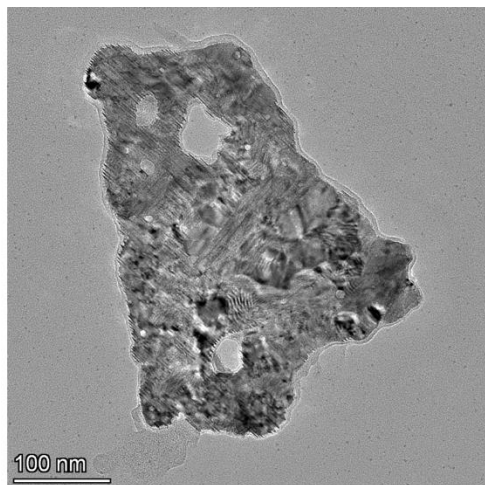


Figure S5 TEM image of Pt-Mo/AC

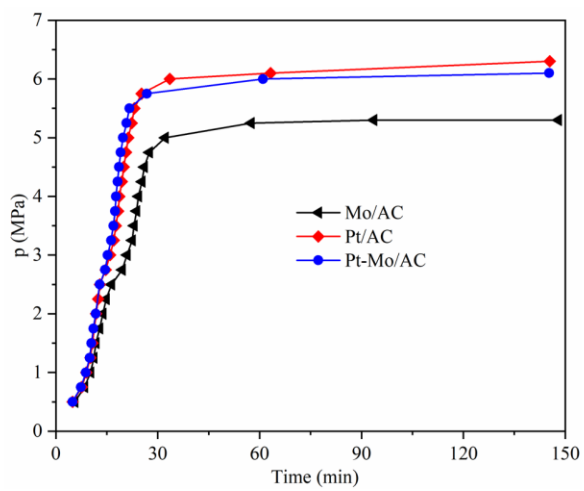


Figure S6. FA decomposition of Mo/AC, Pt/AC and Pt-Mo/AC

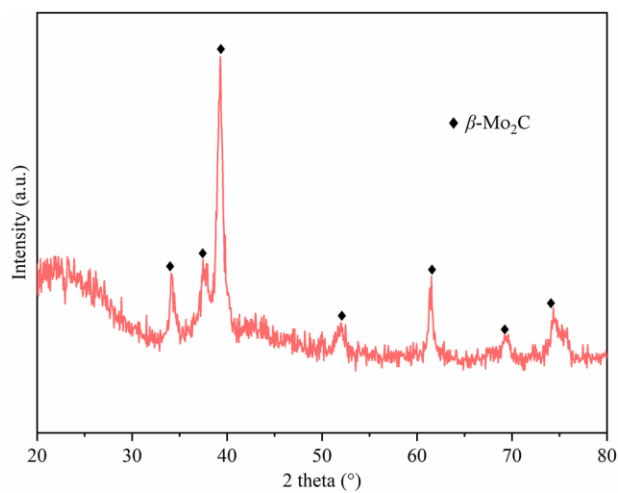


Figure S7. XRD patterns of Pt/Mo/AC

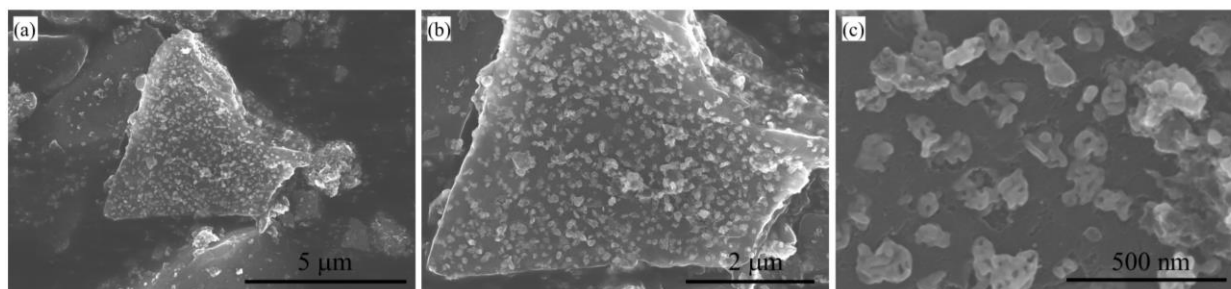


Figure S8. SEM images of Pt/Mo/AC (a-c)

Table S1. Control experiments of in-situ hydrogenation of methyl stearate on different catalysts ^a

Entry	Catalysts	Conv. (%)	Yield (%)			
			Heptadecane	Octadecane	Paraffins (C15-C16)	Others ^b
1	none	7.4	0	0	0	0
2	AC	57.0	3.0	0.6	0	4.2
3	Pt-Mo/AC ^c	85.9	41.3	34.7	0.4	0

^a Reaction conditions: 0.67 mmol methyl stearate, FA/methyl stearate ratio of 38.9, 200 mg catalyst, 20 ml hexane, 290 °C, 2 h. ^b Total yield of hexadecanol, heptadecanol, octadecanol and octadecanal. ^c Reaction conditions: 0.2 MPa H₂

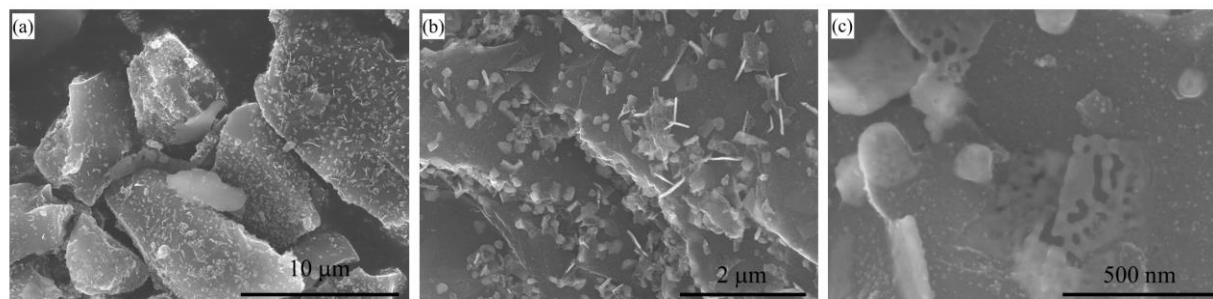


Figure S9. SEM image of used Pt-Mo/AC

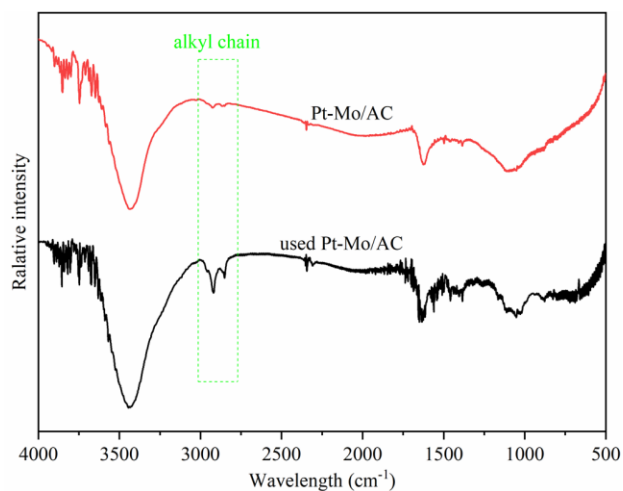


Figure S10. FTIR spectra of Pt-Mo/AC and used Pt-Mo/AC

Table S2. ICP-OES results of the catalysts

Entry	Catalysts	Pt Theoretical loading (wt.%)	Actual loading (wt.%)	
			Pt	Mo
1		0	0	9.3
2		0.2	0.05	7.79
3	Pt-Mo/AC	0.5	0.17	9.04
4		1	0.45	10.03
5		1.5	0.73	9.12
6	Reused Pt-Mo/AC	1	0.29	7.23

Table S3. In-situ hydrogenation of various feedstock over Pt-Mo/AC

Entry	Feedstock	Yield (%)			
		Heptadecane	Octadecane	Paraffins (C15-C16)	Others
1	Stearic acid	70.0	9.3	1.1	4.1
2	Oleic acid	50.9	7.6	7.4	0
3	Ethyl stearate	33.1	9.8	0.3	2.3
4	Corn oil	14.0	1.9	2.8	4.5
5	Biodiesel	16.6	6.1	4.5	0

Reaction conditions: 200 mg feedstock , FA/methyl stearate ratio of 3.9, 200 mg catalyst, 20 ml hexane, 290 °C, 2 h