Supporting Information

Upgrading of palmitic acid to *iso*-alkanes over bi-functional Mo/ZSM-22 catalysts

Yanchun Shi,[a] Yaya Cao,[a] Yanan Duan,[a] Hao Chen,[a] Yu Chen,[a]Mingde Yang,[a]

Yulong Wu[a,b*]

a: Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, PR China

b: Beijing Engineering Research Center for Biofuels, Beijing 100084, China

*Corresponding author: Associate Prof. Yulong Wu

Address: Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, PR China

Tel: +86 010-89796086; Fax: + 86 10-69771464

E-mail: wylong@tsinghua.edu.cn(Y. L. Wu)

Figure captions:

Fig. S1 XRD patterns of commercial MoO_3 (a) and MoO_2 (b)

Fig. S2 Nitrogen isotherms of calcined zeolitic supports K/H-ZSM-22 (A-a and B-a) and Mo/ZSM-22 catalysts before (A-b and B-b) and after reduction (A-c and B-c)

Fig. S3 HRTEM images of calcined zeolitic supports K/H-ZSM-22 (a and b) and Mo/ZSM-22 catalysts before (c and d) and after reduction (e and f)

Fig. S4 Gas chromatogram and mass spectrometry of n-hexadecanal

Fig. S5 Gas chromatogram and mass spectrometry of palmitic acid

Fig. S6 Gas chromatogramof deoxygenation of palmitic acid and isomerization of products over Mo/HZ-R catalyst at 260 ^{o}C for 8 h in presence of 4 MPa H_2(A), mass spectrometry of n-hexadecane (B) and n-pentadecane (C)

Table S1 Unit cell parameters of catalysts by XRD analysis

Table S2 XPS analysis of Mo/ZSM-22 catalysts with different Mo content after reduction

Table S3 Upgrading of palmitic acid over Mo/HZ-R with different Mo content at 260 ^{o}C for 4 h in presence of 4 MPa H_2

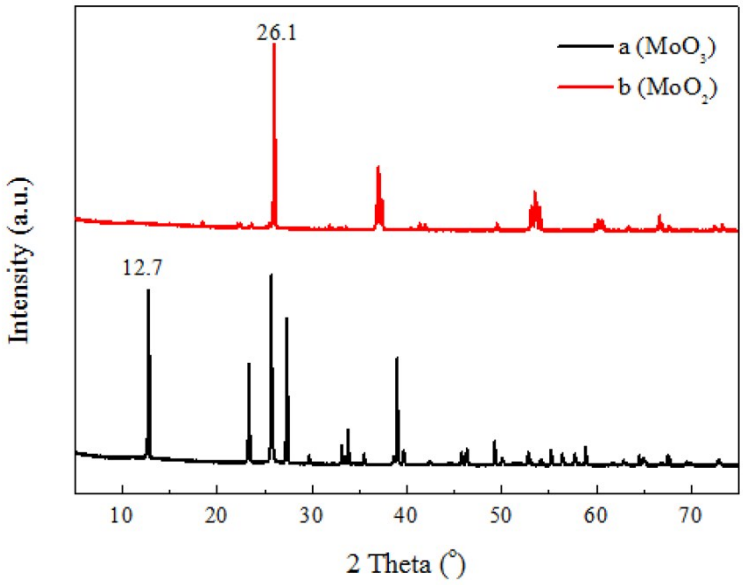

Fig. S1 XRD patterns of commercial MoO_3 (a) and MoO_2 (b)

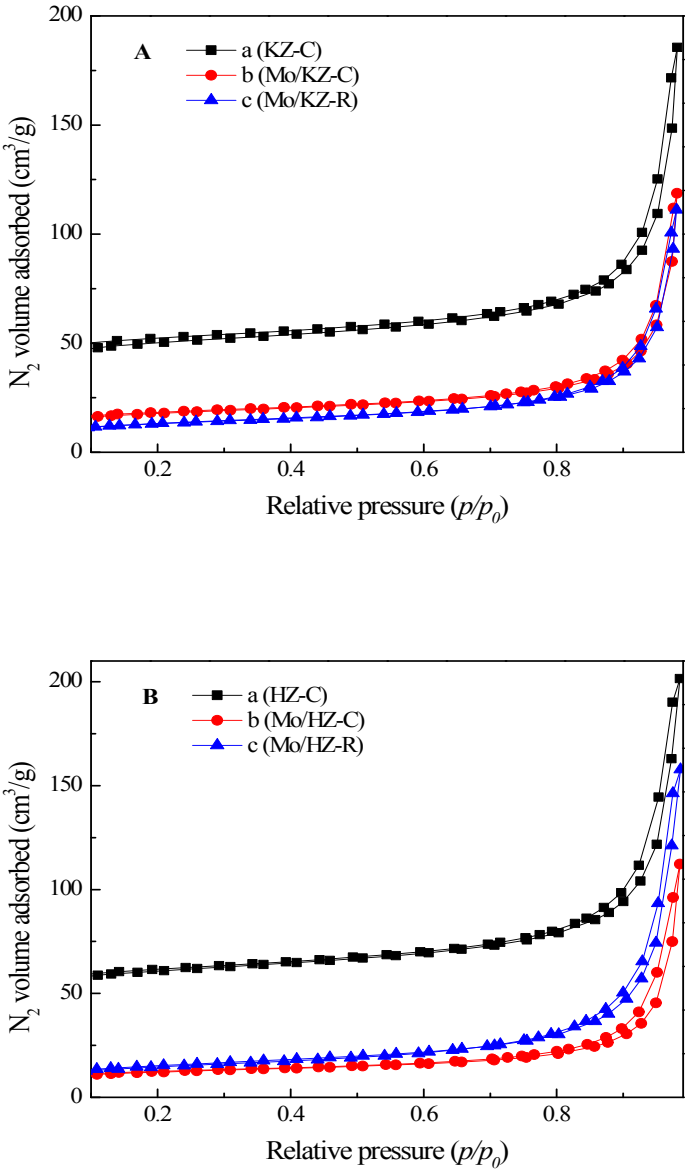

Fig. S2 Nitrogen isotherms of calcined zeolitic supports K/H-ZSM-22 (A-a and B-a) and Mo/TON catalysts before (A-b and B-b) and after reduction (A-c and B-c)

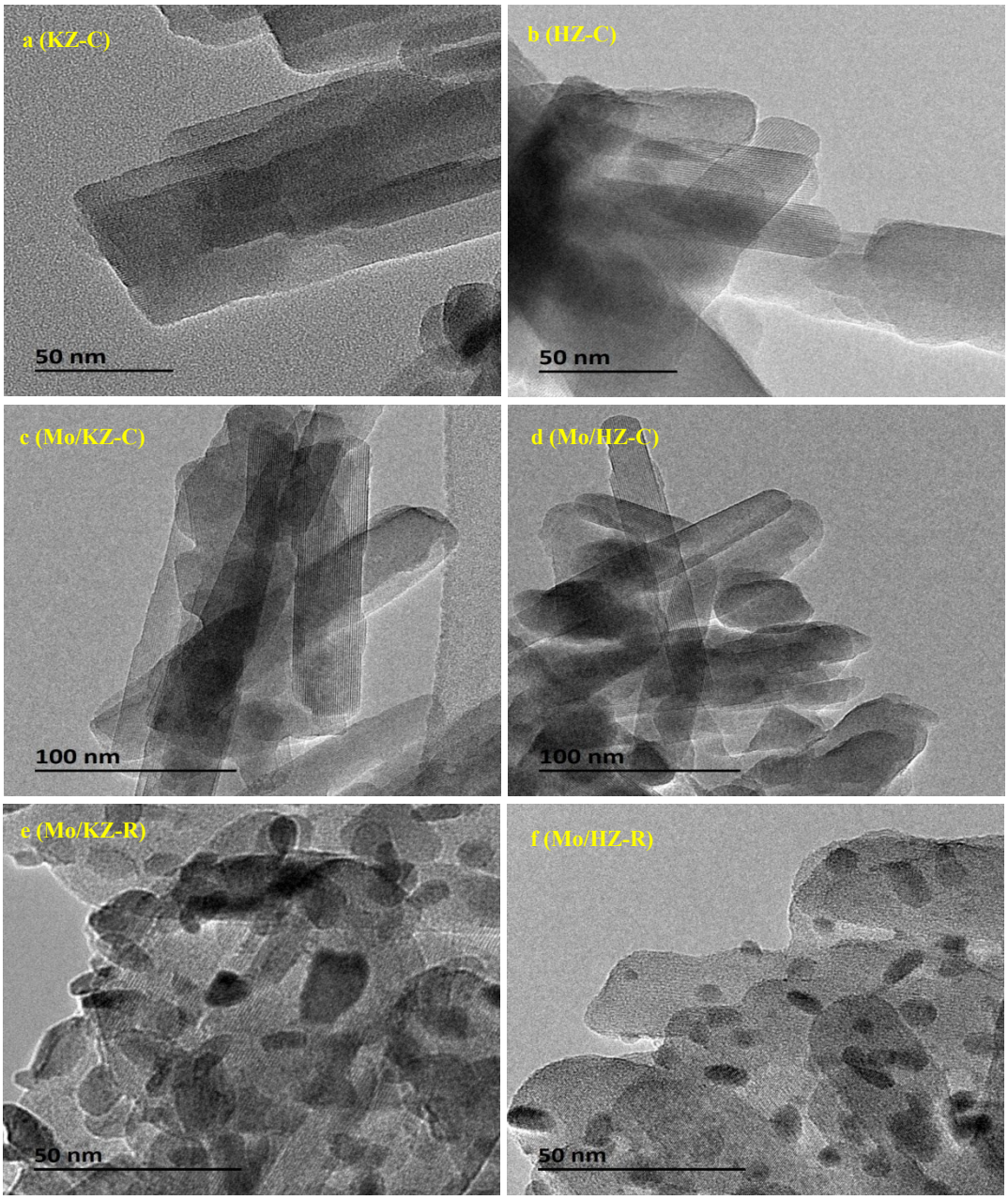

Fig. S3 HRTEM images of calcined zeolitic supports K/H-ZSM-22 (a and b) and Mo/ZSM-22 catalysts before (c and d) and after reduction (e and f)

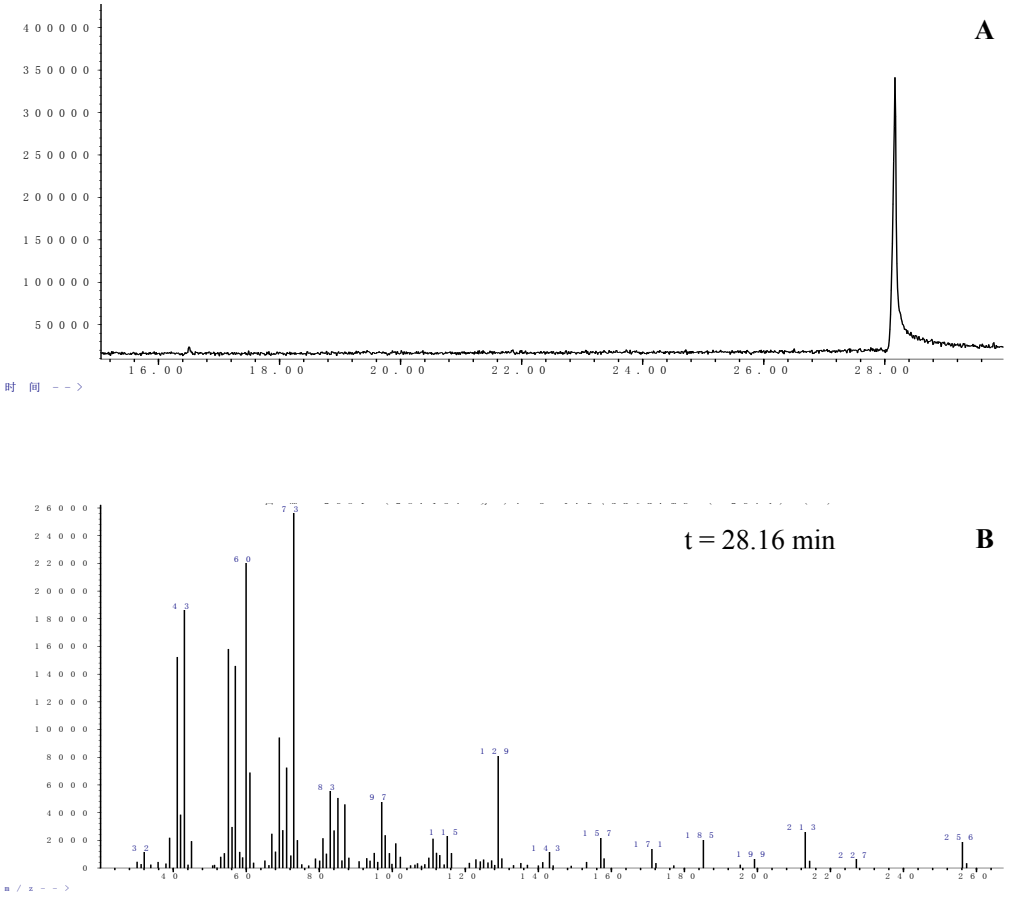

Fig. S4 Gas chromatogram and mass spectrometry of palmitic acid

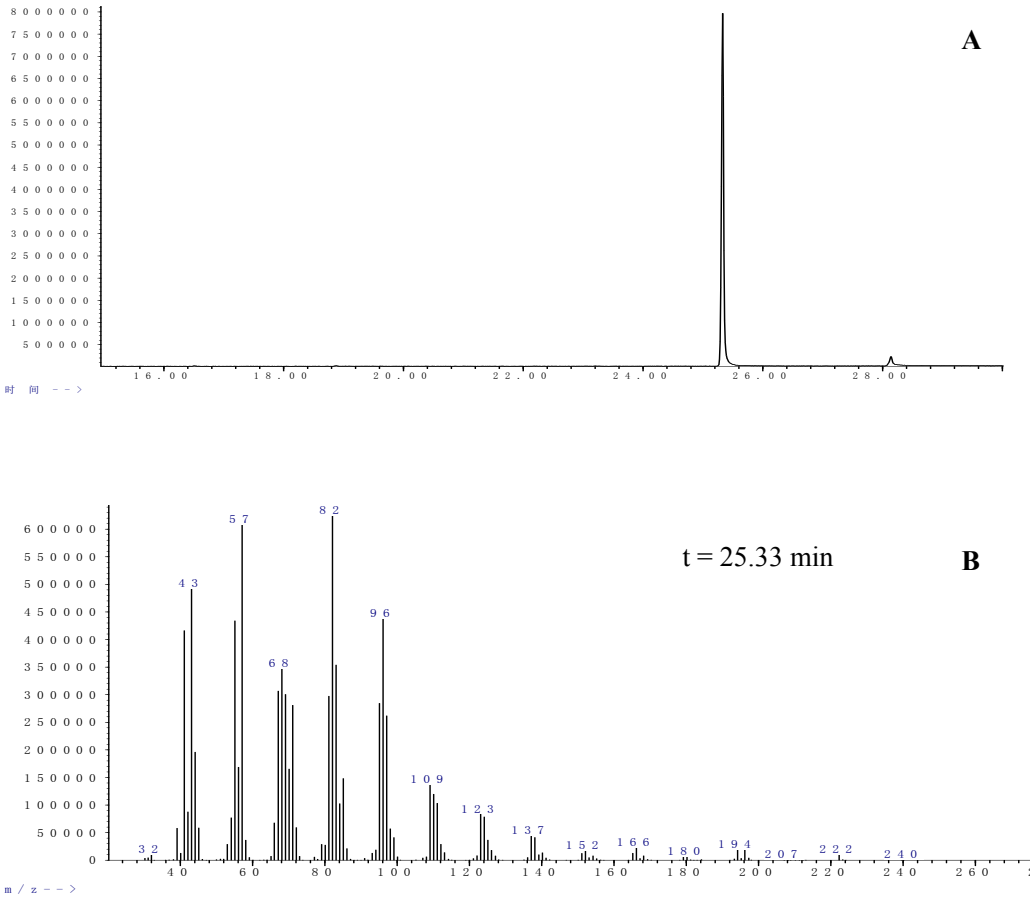

Fig. S5 Gas chromatogram and mass spectrometry of n-hexadecanal

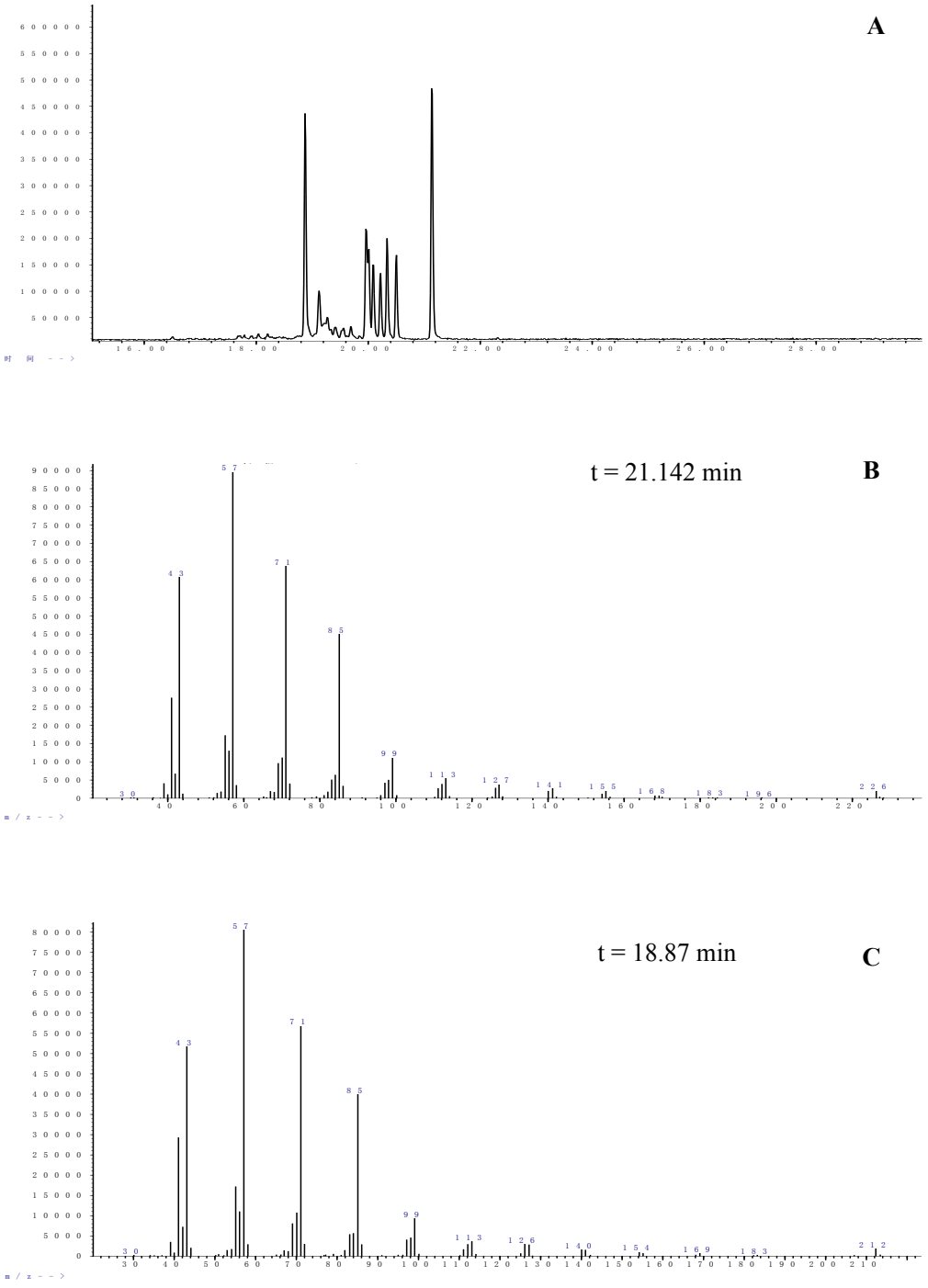

Fig. S6 Gas chromatogramof deoxygenation of palmitic acid and isomerization of products over Mo/HZ-R catalyst at 260 ^{o}C for 8 h in presence of 4 MPa H_2(A), mass spectrometry of n-hexadecane (B) and n-pentadecane (C)

Table S1 Unit cell parameters of catalysts by XRD analysis

Samples	Unit cell parameters of crystals			Volume ($Å^3$)	α/β/γ
	a (Å)	b (Å)	c (Å)	a×b×c	
KZ-C	13.8759	17.4063	5.0378	1216.7701	α = β = γ = 90°
Mo/KZ-C	13.8906	17.4356	5.0406	1220.7876	α = β = γ = 90°
Mo/KZ-R	13.8549	17.2919	5.1086	1223.9085	α = β = γ = 90°
HZ-C	13.8428	17.4038	5.0274	1211.1877	α = β = γ = 90°
Mo/HZ-C	13.9153	17.5184	5.0384	1228.2299	α = β = γ = 90°
Mo/HZ-R	13.9492	17.4910	5.0510	1232.3705	α = β = γ = 90°

Table S2 XPS analysis of Mo/ZSM-22 catalysts with different Mo content after reduction

Catalysts	**Mo/HZ-R-5**	**Mo/HZ-R-10**	**Mo/HZ-R-15**	**Mo/HZ-R**
Mo^{4+}/Mo^{6+}	0.69	0.65	0.62	0.58
Mo/Si	0.02	0.05	0.10	0.15

Table S3 Upgrading of palmitic acid over Mo/HZ-R with different Mo content at 260 °C for 4 h in presence of 4 MPa H_2

Catalysts	**Mo (wt%)**	**Conv. (%)**	**Selectivity (%) of each product after reaction**					
			alkanes	***iso*-C_{16}**	***n*-C_{16}**	***n*-C_{15}**	***n*-C_{14}**	**$C_{15}CHO$**
Mo/HZ-R-1	5	22	66.2	0	6.2	53.3	6.7	33.8
Mo/HZ-R-2	10	67.3	90.3	0	24.3	59.4	6.6	9.7
Mo/HZ-R-3	15	100	61.4	22.4	19.5	19.5	0	38.6
Mo/HZ-R	20	100	100	59.7	15.8	23.6	0.9	0