Supporting Information

Tungsten-doped molybdenum sulfide with dominant double-layer structure on mixed MgAl oxide for higher alcohol synthesis in CO hydrogenation

Xuebin Luan, Jiaxi Yong, Xiaoping Dai,* Xin Zhang, Hongyan Qiao, Yang Yang, Huihui Zhao, Wenyu Peng and Xingliang Huang

State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, China

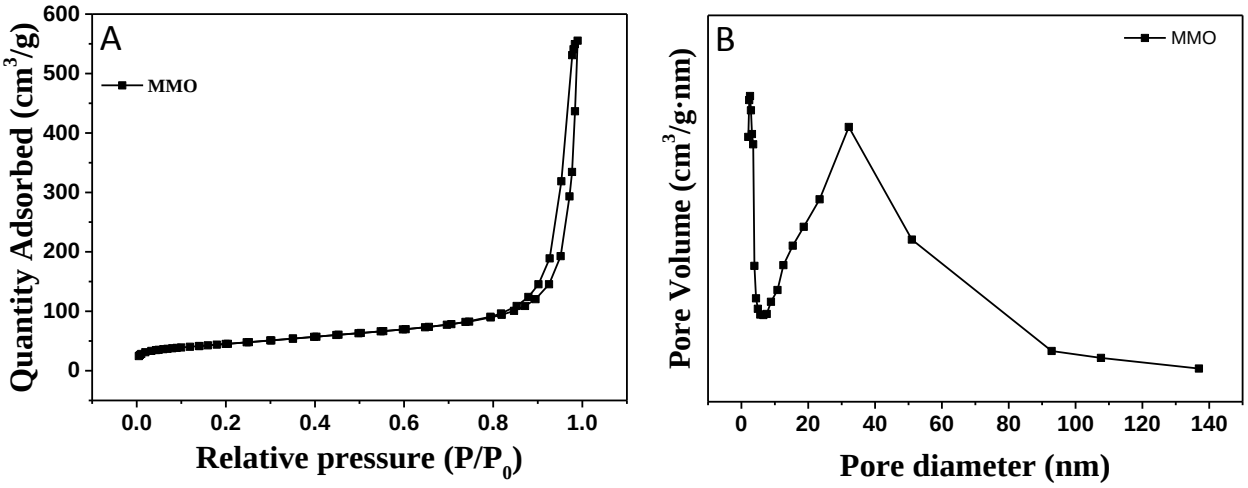


Figure S1. N_2 adsorption–desorption isotherms (A), and pore size distribution (B) for MMO.

Table S1. Surface area and average pore size for support and oxidic catalysts

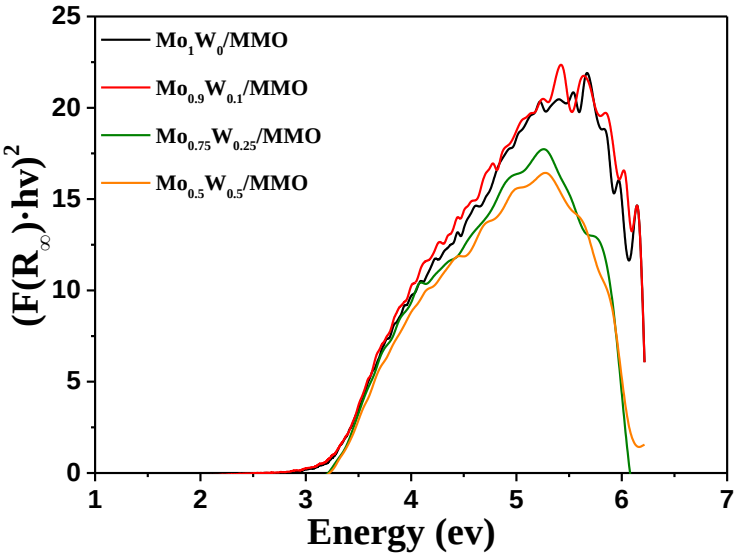
Samples	BET surface area (m^2/g)	Average pore size (nm)	Pore volume (cm^3/g)
MMO	159.3	21.57	0.872
K,Ni-Mo_1W_0/MMO	109.9	5.71	0.184
K,Ni-$Mo_{0.9}W_{0.1}$/MMO	106.8	6.41	0.187
K,Ni-$Mo_{0.75}W_{0.25}$/MMO	121.5	6.02	0.183
K,Ni-$Mo_{0.5}W_{0.5}$/MMO	127.8	5.50	0.207

Table S2 Nominal composition and ICP-MS results of oxidic catalysts

	Catalysts	K (wt. %)	Ni (wt. %)	Mo (wt. %)	W (wt. %)	Mo/(Mo+W) molar ratio	Loading[a] ($at._M/nm^2$)
ICP-MS	K,Ni-Mo_1W_0/MMO	8.37	2.09	6.43	0.04	1.00	2.53
	K,Ni-$Mo_{0.9}W_{0.1}$/MMO	8.87	2.00	5.19	0.89	0.92	2.23
	K,Ni-$Mo_{0.75}W_{0.25}$/MMO	8.86	2.13	4.31	2.66	0.76	2.25
	K,Ni-$Mo_{0.5}W_{0.5}$/MMO	9.37	1.93	2.72	4.8	0.52	2.06
Nominal composition	K,Ni-Mo_1W_0/MMO	8.13	2.03	6.65	0.00	1.00	2.62
	K,Ni-$Mo_{0.9}W_{0.1}$/MMO	8.09	2.02	5.95	1.26	0.9	2.60
	K,Ni-$Mo_{0.75}W_{0.25}$/MMO	8.02	2.01	4.91	3.14	0.75	2.58
	K,Ni-$Mo_{0.5}W_{0.5}$/MMO	7.90	1.97	3.23	6.19	0.5	2.54

[a] The loading ($at._M/nm^2$) was calculate by the following equation.

$$\text{Loading} = \frac{\text{the numbers of atom of W and Mo of catalyst}}{\text{the surface area of supporting}}$$



FigureS2 UV-vis DRS spectra in which the spectrum of MMO has been subtracted of $Mo_{1-x}W_x$/MMO.

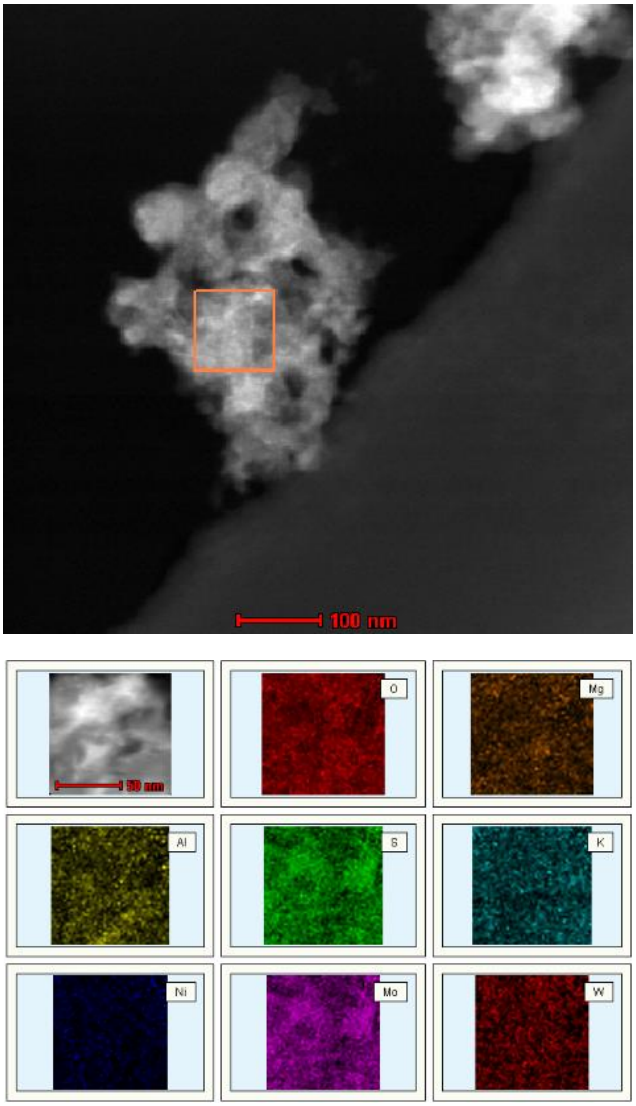


Figure S3 HAADF-STEM images and element mappings of K,Ni-$Mo_{0.75}W_{0.25}S_2$/MMO.

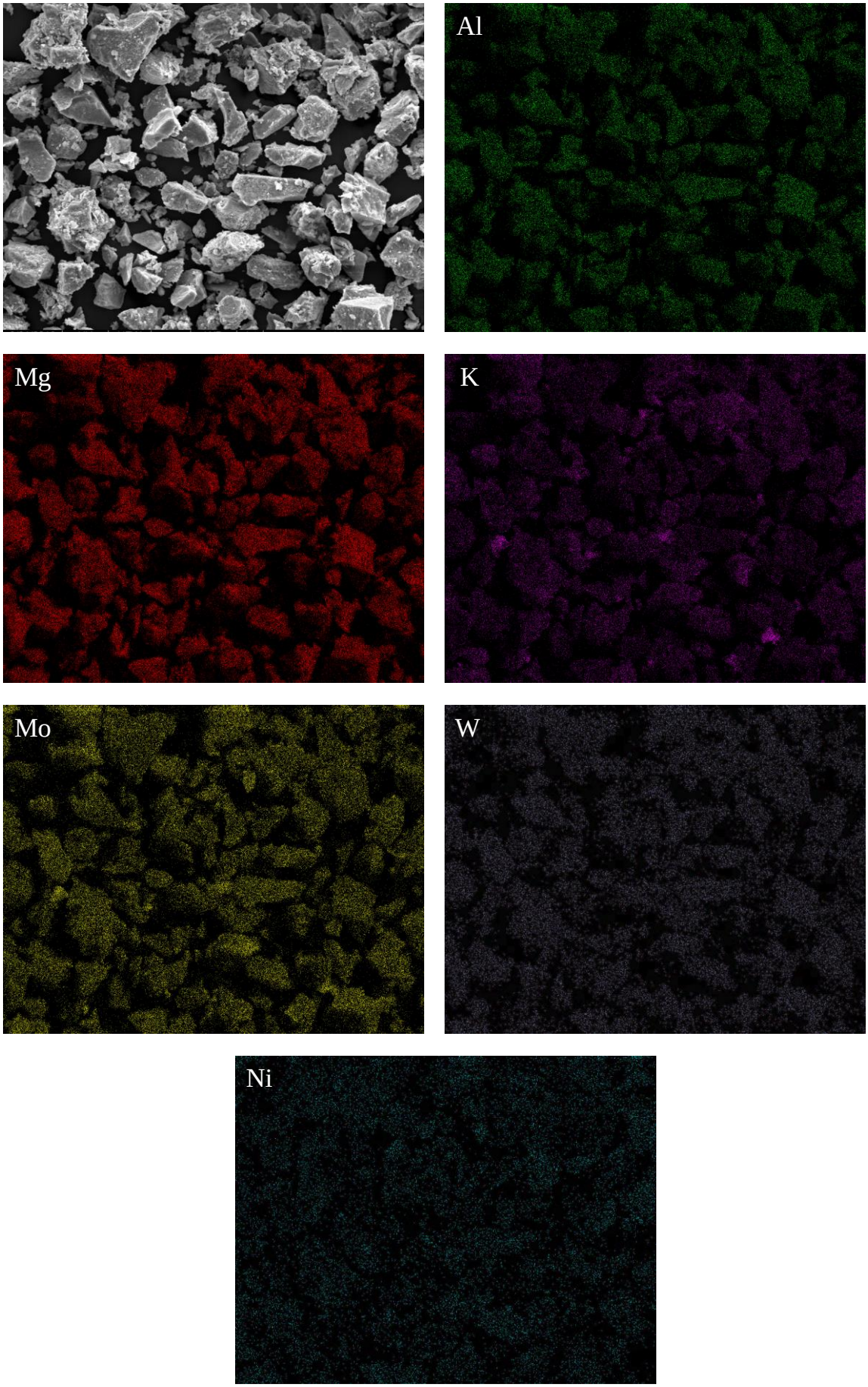


Figure S4 FESEM images and correspond element mappings of K,Ni-$Mo_{0.75}W_{0.25}S_2$/MMO.

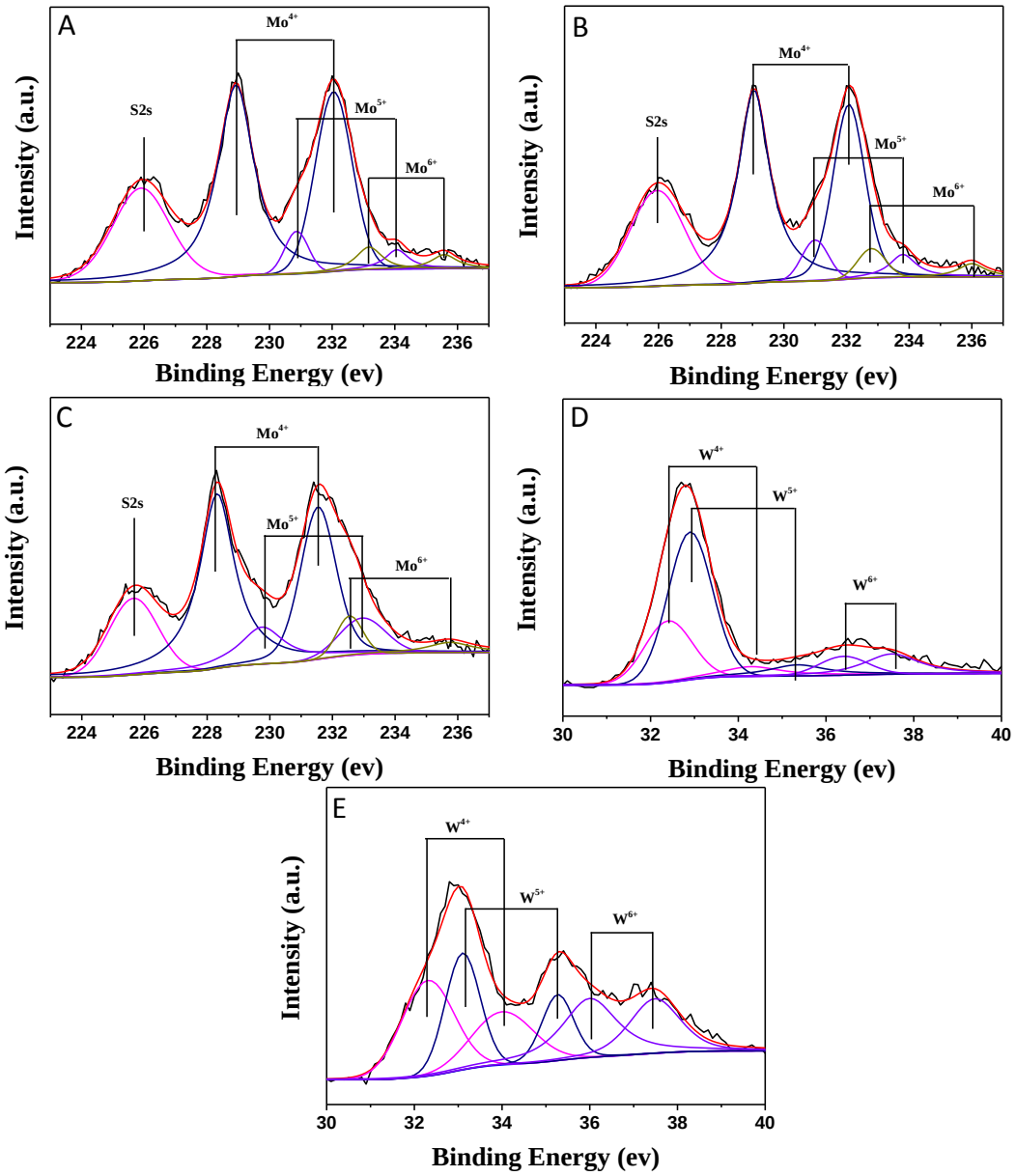


Figure S5 Mo3d XPS spectra of (A) K,Ni-$Mo_1W_0S_2$/MMO, (B) K,Ni-$Mo_{0.9}W_{0.1}S_2$/MMO, (C) K,Ni-$Mo_{0.5}W_{0.5}S_2$/MMO and W4f XPS spectra of (D) K,Ni-$Mo_{0.9}W_{0.1}S_2$/MMO, (E) K,Ni-$Mo_{0.5}W_{0.5}S_2$/MMO.

Table S3 Carbon monoxide hydrogenation on K-$Mo_{1-x}W_xS_2$/MMO.

Catalyst		K-Mo_1W_0/MMO	K-$Mo_{0.9}W_{0.1}$/MMO	K-$Mo_{0.75}W_{0.25}$/MMO	K-$Mo_{0.5}W_{0.5}$/MMO
Conversion （%）		5.8	5.9	5.1	4.8
Selectivity （C%）	Methane	14.9	16.3	16.6	17.1
	Ethane	1.5	1.8	2.7	2.7
	Propane	0.5	0.6	0.7	0.7
	Methanol	12.4	10.5	11.1	12.4
	Ethanol	29.4	29.5	26.7	29.8
	Propanol	16.4	17.1	15.7	12.9
	Butanol	2.1	2.4	4.1	3.0
	other oxygenates	4.2	3.8	3.9	5.5
	Total hydrocarbon	17.0	18.8	20.2	20.6
	Total alcohol	60.2	59.5	57.5	58.1
	CO_2	18.6	18.6	18.4	15.8

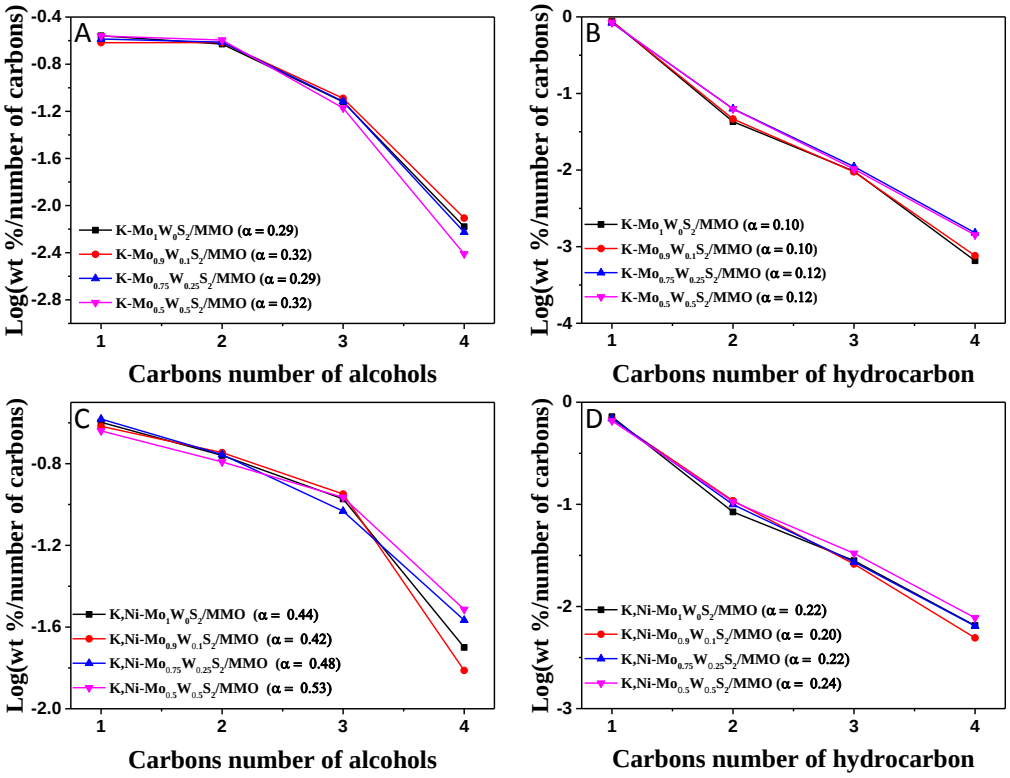


Figure S6. The ASF distribution of (A) hydrocarbon, (B) alcohols on K-$Mo_{1-x}W_xS_2$/MMO catalysts, and (C) hydrocarbon, (D) alcohols on K,Ni-$Mo_{1-x}W_xS_2$/MMO catalysts.