Supporting Information

Mechanistic study of ethanol steam reforming on TM-Mo_6S_8: a DFT study

Zijun Hao, [ab] Ling Guo, *[ab] Minmin Xing [ab] and Qian Zhang [ab]

a. Key Laboratory of Magnetic Molecules & Magnetic Information Materials Ministry of Education, Shanxi Normal University. Linfen, China, 041004.

b. The School of Chemical and Material Science, Shanxi Normal University, No. 1, Gongyuan Street, Linfen, China, 041004.

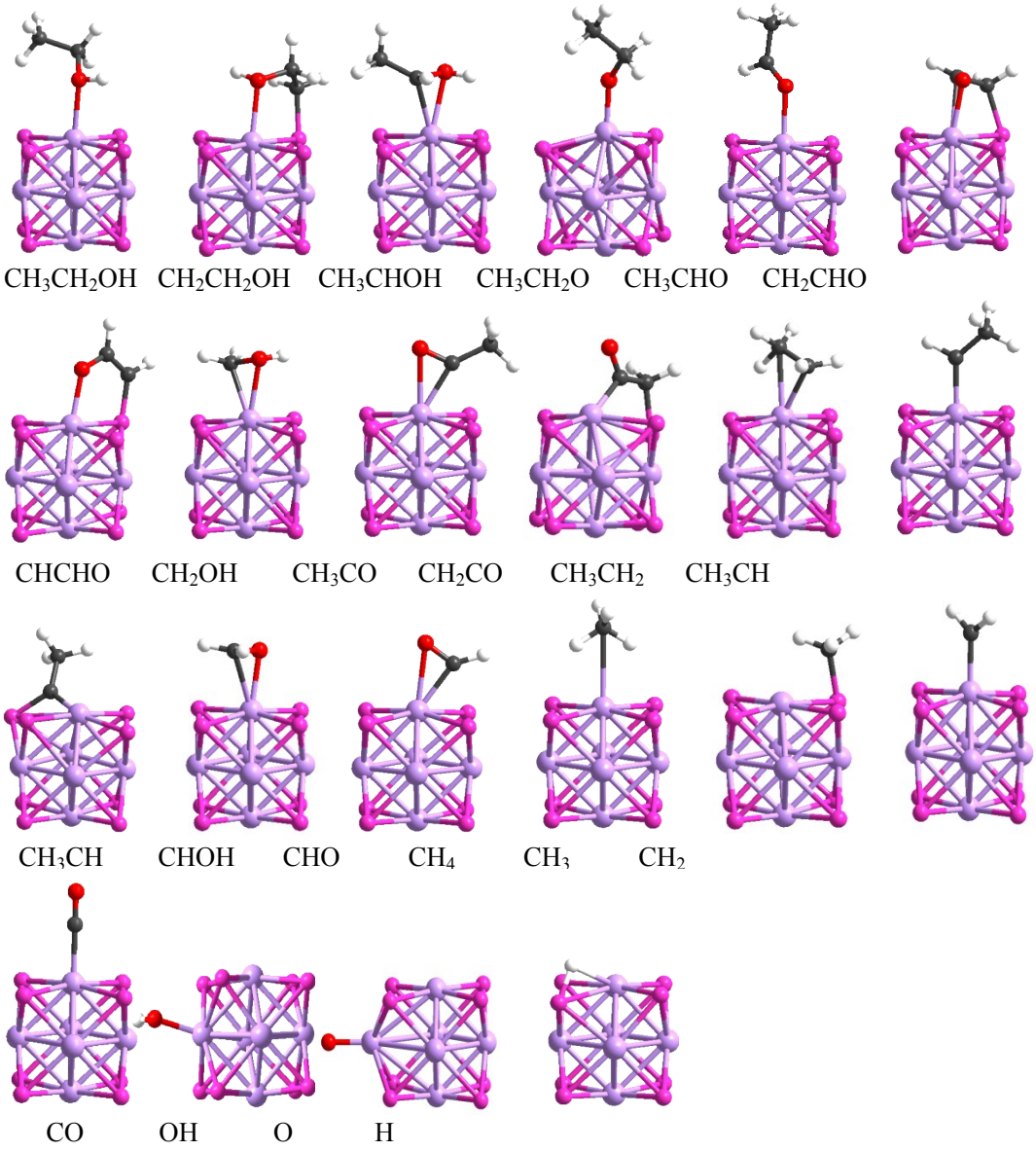

Figure. S1 Adsorption geometries of pertinent species on Mo_6S_8. Atom colors are Mo (purple), S (Pink), O (red), C (black), and H (white).

Table S1 Calculated adsorption energies (E_{ads}) and key geometrical parameters of pertinent species on Mo_6S_8.

Species	E_{ads} (kcal/mol)	preferred adsorption site	Key parameter (Å)
CH_3CH_2OH*	-24.32	Mo-top via O	Mo-O:2.279
CH_3CHOH*	-36.58	Mo-top via C and O	Mo-C:2.301;Mo-O:2.326
CH_2CH_2OH*	-53.41	Mo-S bridge via C and O	S-C:1.869; Mo-O:2.276
CH_3CH_2O*	-45.59	Mo-top via O	Mo-O:1.901
CH_2CH_2O*	-24.81	Mo-S bridge via C and O	S-C:1.856; Mo-O:1.916
CH_3CHO*	-23.69	Mo-top via O	Mo-O:2.216
CH_2CHO*	-31.74	Mo-S bridge via C and O	S-C:1.922; Mo-O:2.199
CH2OH*	-40.32	Mo-top via C and O	Mo-C:2.221; Mo-O:2.283
CH_3CO*	-40.23	Mo-top via C and O	Mo-C:2.131; Mo-O:2.348
CH_2CO*	-4.49	Mo-S bridge via C	Mo-C:2.066;S-C:1.850
CH_2O*	-15.31	Mo-top via C and O	Mo-C:2.429; Mo-O:2.175
CH_3CH_2*	-30.80	Mo-top via C	Mo-C_1:2.267; Mo-C_2:2.487
CH_3CH*	-71.03	Mo-top via C	Mo-C:2.035
CH_3C*	-98.35	S-Mo bridge via C	S-C:1.745; Mo-C:2.101
CHO*	-37.44	Mo-top via C and O	Mo-C:2.109; Mo-O:2.435
CH_4*	-4.80	Mo-top via C	Mo-C:2.831
CH_3*	-36.22	Mo-S bridge via C	S-C:1.871; Mo-C:2.859
CH_2*	-78.04	Mo-top via C	Mo-C:2.002
CO*	-33.61	Mo-top via C	Mo-C:2.081
OH*	-60.30	Mo-top via O	Mo-C:1.936
H*	-46.88	S-Mo bridge via H	S-H:1.3899; Mo-H:2367
O*	-421.20	Mo-top via O	Mo-O:1.709