

A Thoroughly Mechanistic Study of Ethanol, Acetaldehyde, and Ethylene Adsorption on Cu-MOR via DFT Analysis

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Table S1. Geometric parameters of Cu₃/MOR, Cu₃O₃/MOR and Cu₆/MOR before and after adsorption.

	Before adsorption	CH ₃ CH ₂ OH adsorption	CH ₃ CHO adsorption	CH ₂ CH ₂ adsorption
Cu ₃ /MOR				
d (Cu1-Cu2) (Å)	2.338	2.337	2.326	2.322
d (Cu1-Cu3) (Å)	2.262	2.319	2.382	2.404
d (Cu2-Cu3) (Å)	2.322	2.260	2.314	2.444
d (Cu1-O1) (Å)	2.042	2.048	1.991	1.965
d (Cu1-O2) (Å)	2.439	2.461	2.631	2.884
d (Cu2-O3) (Å)	2.047	2.048	2.054	2.044
d (Cu2-O4) (Å)	2.079	2.091	2.128	2.094
d (Cu3-O5) (Å)	2.052	2.056	2.319	2.136
d (Cu3-O6) (Å)	2.105	2.140	2.287	2.480
Cu ₃ O ₃ /MOR				
d (Cu1-O1) (Å)	1.776	1.780	1.775	1.793
d (Cu1-O2) (Å)	1.821	1.831	1.818	1.978
d (Cu2-O2) (Å)	1.794	1.810	1.797	1.981
d (Cu2-O3) (Å)	1.776	1.779	1.781	1.959
d (Cu3-O1) (Å)	1.812	1.808	1.813	1.817
d (Cu3-O3) (Å)	1.792	1.788	1.802	1.903
d (Cu1-O4) (Å)	2.440	2.460	2.423	2.752
d (Cu1-O5) (Å)	2.006	2.004	2.004	2.004
d (Cu2-O6) (Å)	2.042	2.034	2.020	2.115
d (Cu2-O7) (Å)	2.098	2.097	2.088	2.097
d (Cu3-O8) (Å)	2.031	2.022	2.028	2.069
d (Cu3-O9) (Å)	1.974	1.968	1.982	2.007
Cu ₆ /MOR				
d (Cu1-Cu2) (Å)	2.367	2.342	2.360	2.356
d (Cu1-Cu3) (Å)	2.489	2.493	2.507	2.488

d (Cu2-Cu3) (Å)	2.443	2.453	2.423	2.417
d (Cu3-Cu4) (Å)	2.434	2.370	2.369	2.376
d (Cu4-Cu5) (Å)	2.338	2.321	2.304	2.324
d (Cu5-Cu6) (Å)	2.375	2.375	2.403	2.414
d (Cu4-Cu6) (Å)	2.446	2.494	2.510	2.520
d (Cu2-Cu6) (Å)	2.479	2.429	2.501	2.547
d (Cu3-Cu6) (Å)	2.334	2.354	2.399	2.392
d (Cu2-Cu5) (Å)	2.527	2.582	2.489	2.486
d (Cu6-Cu1) (Å)	2.423	2.478	2.423	2.431
d (Cu2-O1) (Å)	2.003	2.005	2.010	2.016
d (Cu3-O2) (Å)	2.051	2.167	2.199	2.094
d (Cu4-O3) (Å)	2.010	2.004	1.980	2.014
d (Cu5-O4) (Å)	2.012	2.023	2.012	2.028

Table S2. Geometric parameters of C₂H₅OH, C₂H₄O, and C₂H₄ species before and after adsorption.

	Free molecule	Adsorbed Cu ₃ /MOR	on Adsorbed Cu ₃ O ₃ /MOR	on Adsorbed Cu ₆ /MOR
C ₂ H ₅ OH				
d (O-H6) (Å)	0.977	0.978	1.000	0.985
d (C2-O) (Å)	1.436	1.446	1.426	1.460
d (C2-H5) (Å)	1.106	1.105	1.102	1.102
d (C2-H4) (Å)	1.100	1.106	1.103	1.092
d (C2-C1) (Å)	1.519	1.515	1.530	1.511
d (C1-H3) (Å)	1.100	1.100	1.099	1.099
d (C1-H2) (Å)	1.098	1.100	1.100	1.096
d (C1-H1) (Å)	1.101	1.100	1.102	1.110
∠(H6-O-C2) (°)	108.063	108.209	110.113	110.682
∠(O-C2-H4) (°)	104.916	110.263	106.133	107.871
∠(O-C2-H5) (°)	110.509	110.024	110.794	109.283
∠(C1-C2-H4) (°)	110.421	110.525	109.285	111.889
∠(C1-C2-H5) (°)	110.487	110.483	110.082	111.344
∠(O-C2-C1) (°)	112.934	107.583	112.126	106.333
∠(C2-C1-H1) (°)	110.581	110.602	110.344	110.923
∠(C2-C1-H2) (°)	110.744	110.628	110.425	110.627
∠(C2-C1-H3) (°)	111.137	110.562	110.036	110.411
C ₂ H ₄ O				
d (C2-O) (Å)	1.224	1.242	1.246	1.288
d (C2-H4) (Å)	1.120	1.110	1.110	1.107
d (C2-C1) (Å)	1.496	1.480	1.472	1.492
d (C1-H3) (Å)	1.096	1.104	1.102	1.104
d (C1-H2) (Å)	1.102	1.106	1.096	1.096
d (C1-H1) (Å)	1.102	1.097	1.110	1.097
∠(O-C2-H4) (°)	120.023	116.996	119.338	118.793

$\angle(\text{C1-C2-H4})$ ($^\circ$)	115.320	118.351	117.280	118.169
$\angle(\text{O-C2-C1})$ ($^\circ$)	124.657	124.652	123.365	121.443
$\angle(\text{C2-C1-H1})$ ($^\circ$)	109.470	109.240	109.870	107.850
$\angle(\text{C2-C1-H2})$ ($^\circ$)	109.483	109.060	111.857	111.627
$\angle(\text{C2-C1-H3})$ ($^\circ$)	111.175	111.682	107.292	110.853
C_2H_4				
d (C1-H1) (\AA)	1.093	1.093	1.103	1.094
d (C1-H2) (\AA)	1.093	1.093	1.098	1.092
d (C2-C1) (\AA)	1.332	1.382	1.551	1.390
d (C2-H3) (\AA)	1.092	1.094	1.104	1.093
d (C2-H4) (\AA)	1.092	1.092	1.100	1.091
$\angle(\text{C1-C2-H3})$ ($^\circ$)	121.591	120.966	111.809	121.029
$\angle(\text{C1-C2-H4})$ ($^\circ$)	121.737	121.300	109.422	121.105
$\angle(\text{H1-C1-H2})$ ($^\circ$)	116.501	121.277	108.590	115.905
$\angle(\text{C2-C1-H1})$ ($^\circ$)	121.700	121.277	109.932	121.053
$\angle(\text{C2-C1-H2})$ ($^\circ$)	121.800	121.021	110.643	120.900
$\angle(\text{H3-C2-H4})$ ($^\circ$)	116.672	115.887	107.846	115.856

Table S3 The Bader charges of Cu_3 , Cu_3O_3 and Cu_6 in MOR.

	Cu_3	Cu_3O_3	Cu_6
Cu1	18.5469	17.8486	18.9972
Cu2	18.5459	17.8856	18.8593
Cu3	18.5939	17.9294	18.7399
O1/Cu4	-	6.76262	18.6146
O2/Cu5	-	6.71623	18.686
O3/Cu6	-	6.74611	18.6819