Adsorption of biomass derived products on MoO_3: Hydrogen bonding interactions under the spotlight

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SUPPORTING INFORMATION

Figure S1. Optimized geometries for the adsorption of palmitic acid on MoO_3 at σ_H = 11 % (A), 33 % (B), 56 % (C) and 78 % (D)

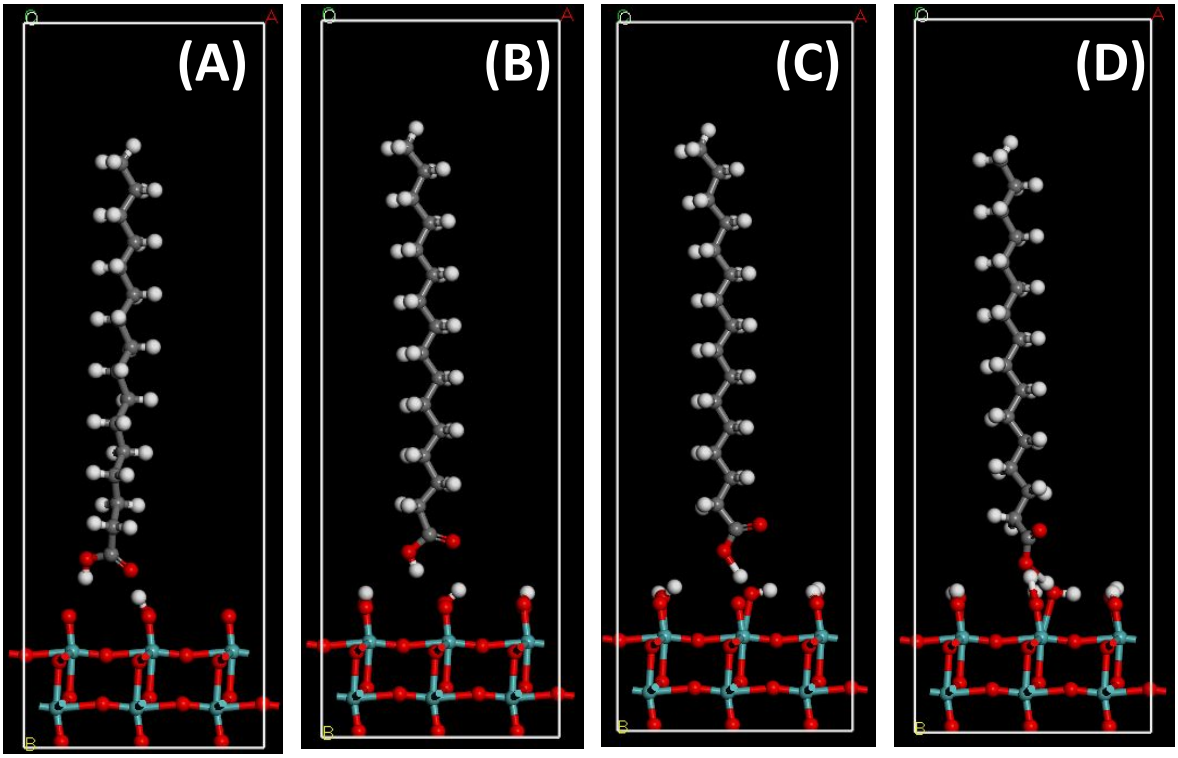


Figure S2. Optimized geometries for the adsorption of m-cresol on MoO_3 at σ_H = 11 % (A), 33 % (B), 56 % (C) and 78 % (D)

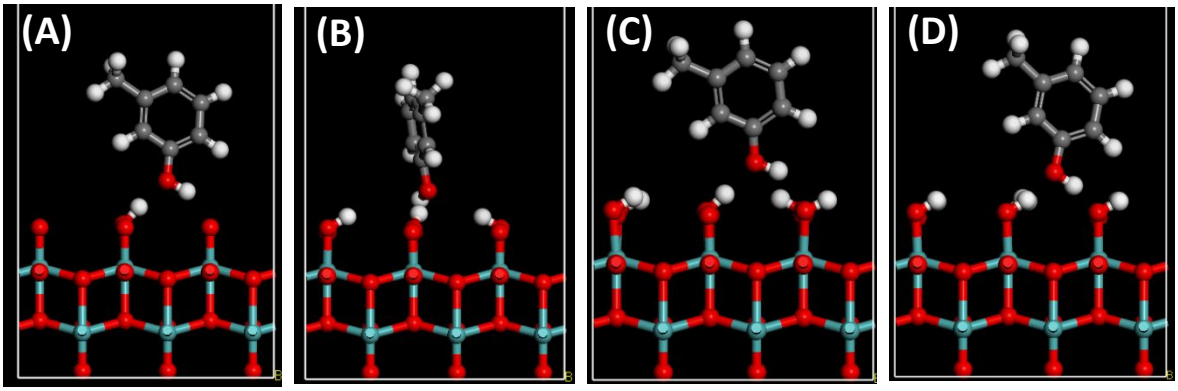


Figure S3. Optimized geometries for the adsorption of guaiacol on MoO_3 at σ_H = 11 % (A), 33 % (B), 56 % (C) and 78 % (D)

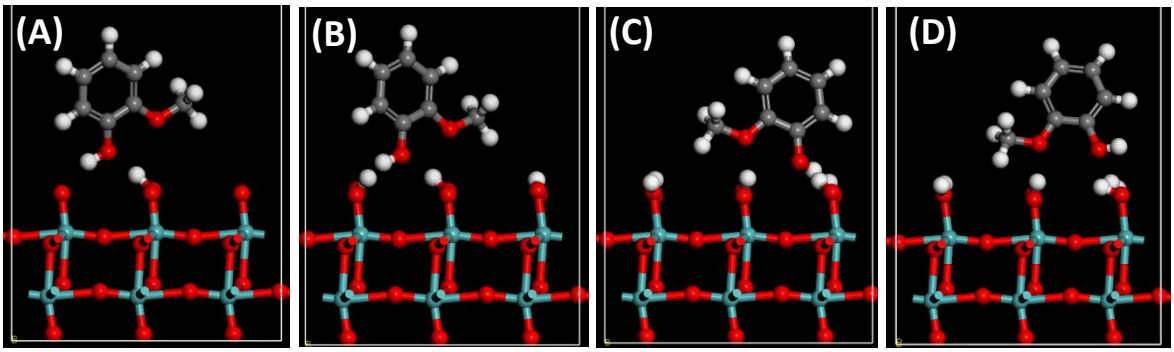
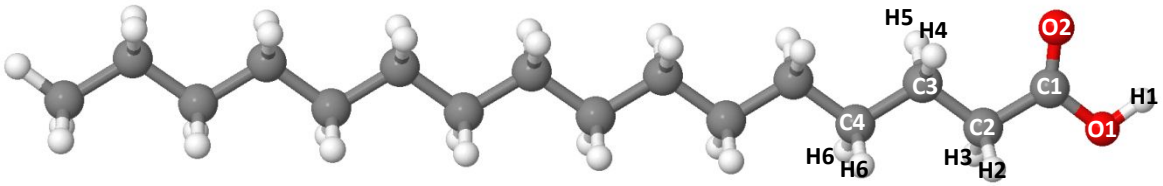


Table S1. Selected bond lengths and angles for the palmitic acid adsorbed on MoO3 surfaces

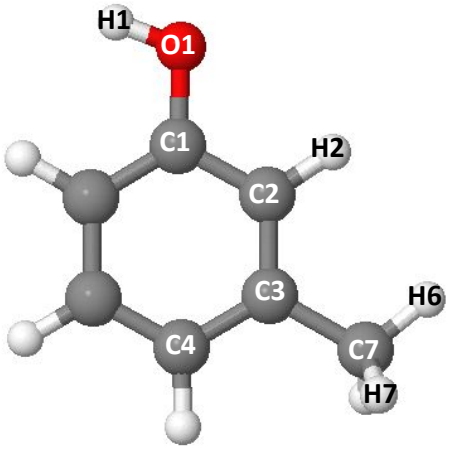
		σ_H (%)					
	Ground state	0	11	33	56	78	100
Bond	**Length (Å)**						
C1-O1	1.35	1.36	1.34	1.37	1.36	1.36	1.36
C1-O2	1.20	1.22	1.24	1.23	1.24	1.24	1.24
C1-C2	1.50	1.52	1.51	1.52	1.51	1.52	1.52
C2-C3	1.52	1.54	1.56	1.52	1.55	1.55	1.55
C3-C4	1.52	1.54	1.54	1.55	1.54	1.54	1.54
O1-H1	0.97	0.98	0.99	0.98	0.99	0.99	0.99
C2-H2	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C2-H3	1.09	1.09	1.09	1.09	1.09	1.09	1.09
Angle	**(°)**						
C1-O1-H1	107.1	107.5	111.3	107.2	108.4	108.5	108.5
O1-C1-O2	122.2	122.6	124.4	122.5	123.2	123.3	123.3
O1-C1-C2	111.8	111.5	112.8	109.8	112.9	112.8	112.8
Dihedral angle	**(°)**						
O2-C1-O1-H1	0.3	0.1	5.7	2.7	0.3	0.6	0.6
C2-C1-O1-H1	179.7	179.3	174.2	176.2	179.8	179.7	179.7
O2-C1-C2-C3	0.4	6.0	99.7	12.5	98.4	98.7	98.7
C1-C2-C3-C4	180.0	180.0	170.8	177.1	180.0	177.4	177.4



Scheme 1. Optimized geometry for palmitic acid and atoms labeling.

Table S2. Selected bond lengths and angles for the m-cresol adsorbed on MoO_3 surfaces

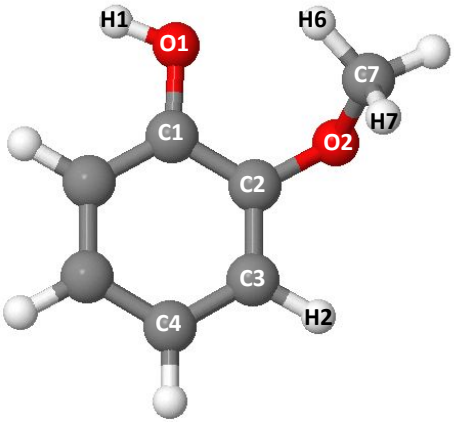
		σ_H (%)					
	Ground state	0	11	33	56	78	100
Bond	**Length (Å)**						
C1-O1	1.36	1.36	1.39	1.40	1.39	1.39	1.39
C1-C2	1.39	1.42	1.40	1.40	1.40	1.41	1.41
C2-C3	1.39	1.40	1.40	1.41	1.41	1.41	1.41
C3-C4	1.40	1.42	1.41	1.41	1.41	1.41	1.41
O1-H1	0.96	0.98	0.98	0.98	0.98	0.98	1.01
C2-H2	1.08	1.09	1.09	1.09	1.09	1.09	1.09
C3-C7	1.50	1.52	1.52	1.52	1.52	1.52	1.52
C7-H6	1.09	1.10	1.10	1.10	1.10	1.10	1.10
Angle	**(°)**						
C1-O1-H1	109.6	110.8	111.0	111.2	112.0	108.0	110.2
O1-C1-C2	117.2	116.3	117.6	117.0	117.1	118.1	117.8
C1-C2-C3	120.5	120.6	120.3	120.1	120.4	120.4	121.1
C2-C3-C7	119.0	121.0	120.9	120.7	120.6	120.8	118.7
Dihedral angle	**(°)**						
H1-O1-C1-C2	179.7	179.6	177.3	166.8	175.1	173.9	155.2
O1-C1-C2-H2	0.1	0.3	1.2	1.3	0.3	1.0	1.8
H2-C2-C3-C7	0.1	0.0	0.3	0.3	0.9	1.7	1.7
C2-C3-C7-H6	2.2	2.2	1.9	0.5	4.1	16.7	24.3



Scheme 2. Optimized geometry for m-cresol and atoms labeling.

Table S3. Selected bond lengths and angles for the guaiacol adsorbed on MoO_3 surfaces

		σ_H (%)					
	Ground state	0	11	33	56	78	100
Bond	**Length (Å)**						
C1-O1	1.36	1.36	1.39	1.39	1.39	1.40	1.39
C1-C2	1.40	1.44	1.43	1.42	1.42	1.42	1.42
C2-C3	1.38	1.41	1.41	1.41	1.41	1.41	1.40
C3-C4	1.39	1.39	1.40	1.41	1.41	1.40	1.41
O1-H1	0.96	0.98	0.99	0.99	0.99	0.97	1.05
C2-O2	1.37	1.36	1.37	1.37	1.38	1.38	1.40
O2-C7	1.42	1.46	1.44	1.44	1.45	1.45	1.45
C3-H4	1.08	1.09	1.09	1.09	1.09	1.09	1.09
C7-H6	1.09	1.10	1.10	1.10	1.10	1.10	1.10
Angle	**(°)**						
C1-O1-H1	109.4	110.7	110.9	110.3	108.9	107.9	112.1
O1-C1-C2	117.6	118.4	116.7	116.7	117.3	117.9	118.4
C1-C2-C3	119.4	118.6	118.7	118.8	119.1	118.8	119.6
C1-C2-O2	120.9	126.7	115.1	114.9	115.2	116.6	116.2
C2-O2-C7	114.5	122.9	118.4	118.7	118.3	117.1	117.1
Dihedral angle	**(°)**						
H1-O1-C1-C2	177.5	177.5	176.9	177.3	139.8	157.9	135.1
O1-C1-C2-O2	1.4	0.5	1.7	2.5	2.6	1.6	1.4
C1-C2-O2-C7	70.9	18.9	179.0	179.7	173.4	163.2	173.1
O2-C2-C3-H2	1.8	1.2	0.4	0.4	1.4	1.1	0.5



Scheme 3. Optimized geometry for guaiacol and atoms labeling.