

Electronic Supplementary Information

Ab initio study of methanol and ethanol adsorption on Brønsted sites in zeolite H-MFI

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S1. Additional Hybrid MP2/CPC-CBS:PBE+D2 results

Table S1. $H_z \cdots O_a$ (R_1), $O_z H_z$, $H_a \cdots O_z$ (R_2), and $O_a H_a$ distances for the PBE+D2 and MP2/CPC-CBS(D,T):PBE+D2 structures, in pm.

	R_1	$O_z H_z$	$O_z H_z^a$	R_2	$O_a H_a$	$O_a H_a^b$
<i>Methanol</i>						
PBE+D2	134.1	111.9	97.7	196.2	98.9	97.2
MP2/CPC-CBS(D,T):PBE+D2	145.8	104.2	96.4	209.9	96.9	95.6
<i>Ethanol</i>						
PBE+D2	131.5	113.7		198.8	98.9	97.3
MP2/CPC-CBS(D,T):PBE+D2	145.0	104.5		213.7	97.0	96.0

^a Unloaded zeolite; ^b alcohol in the gas phase ¹

Table S2. Hybrid MP2/CPC-CBS(T,Q):PBE+D2+ Δ CCSD(T) adsorption energies of methanol and ethanol onto H-ZSM-5 zeolite, in kJ/mol. All the calculations are performed at the MP2/CPC-CBS(D,T):PBE+D2 equilibrium structures.

	Methanol	Ethanol
PBE+D2 (pbc)	-117.08	-132.66
PBE+D2 (C)	-115.47	-124.80
MP2/CPC-CBS(T,Q) (C)	-100.51	-106.00
Δ_{LR}	-1.61	-7.86
Δ_{HL}	14.96	18.79
MP2/CPC-CBS(T,Q):PBE+D2	-102.12	-113.87
CCSD(T)-MP2 ^a	1.42	1.10
MP2/CPC-CBS(T,Q):PBE+D2+ Δ CCSD(T) ^a	-100.70	-112.77

^a CCSD(T) corrections to the MP2 results are computed for smaller cluster (3T) and T-zeta basis set.

Table S3. $R_1(\text{OH}\cdots\text{OH}(\text{C}))$ and $R_2(\text{O}\cdots\text{HO}(\text{C}))$ distances, in pm, and adsorption energies, in kJ/mol, obtained with hybrid MP2/CPC-CBS(D,T):PBE+D2 and hybrid MP2/CPC-CBS(T,Q):PBE+D2.

	Methanol			Ethanol		
	(D,T) ^a	(T,Q) ^a	(T,Q) ^b	(D,T) ^a	(T,Q) ^a	(T,Q) ^b
PBE+D2 (pbc)	-117.08		-117.49	-132.66		-133.76
PBE+D2 (C)	-115.47		-114.96	-124.80		-126.46
MP2 (C)	-97.22	-100.51	-98.96	-103.17	-106.00	-105.76
Δ_{LR}	-1.61		-2.53	-7.86		-7.29
Δ_{HL}	18.25	14.96	16.00	21.62	18.79	20.71
MP2:PBE+D2	-98.83	-102.12	-101.50	-111.03	-113.87	-113.05
R_1	145.8		144.5	145.0		142.4
R_2	209.9		212.8	213.7		217.2

^a Calculations are performed at the MP2/CPC-CBS(D,T):PBE+D2 equilibrium structures.

^b Calculations are performed at the MP2/CPC-CBS(T,Q):PBE+D2 equilibrium structures.

S2. Additional thermodynamic results

Table S4. Standard Gibbs free energy, ΔG , standard entropy term, $-T\cdot\Delta S$, and its translational, rotational and vibrational contributions for the adsorption of methanol and ethanol in H-MFI, all in kJ/mol. Standard entropy, ΔS , in J/(mol·K.)

	Methanol ^a		Ethanol ^b			
	This work		This work		Alexopoulos et al. ²	
	HA	AnHA	HA	AnHA	HA	QHA
ΔG ^c	-41.1	-27.7	-53.2	-56.0	-74	-44±6
$-T\cdot\Delta S$	58.8	55.7	60.9	48.0	51.9	63±5
$-T\cdot\Delta S_{tra}$	45.7	45.7	47.0	47.0	47.1	35.4
$-T\cdot\Delta S_{rot}$	35.2	35.2	36.7	36.7	28.5	29.4
$-T\cdot\Delta S_{vib}$	-22.1	-25.2	-22.8	-35.7	-23.4	1.5
ΔS	-196.0	-185.7	-203.0	-160.0	-173.0	-210.0±16.7
ΔS_{tra}	-152.3	-152.3	-156.7	-156.7	-157.0	-118.0
ΔS_{rot}	-117.3	-117.3	-122.3	-122.3	-95.0	-98.0
ΔS_{vib}	73.7	84.0	76.0	119.0	78.0	-5.0
K_{eq} ^d	1.4×10^7	6.5×10^4	1.8×10^9	5.3×10^9	7.2×10^{12}	4.4×10^7

Table S5. Harmonic and anharmonic enthalpies, ΔH , entropy terms, $-T^*\Delta S$, and Gibbs free energies, ΔG , in kJ mol⁻¹, as well as entropies, ΔS , in kJ mol⁻¹ K⁻¹ for the adsorption of ethanol on H-ZSM-5 at 200, 300, and 400 K.

T	Harmonic				Anharmonic			
	ΔH	$-T\Delta S$	ΔS	ΔG	ΔH	$-T\Delta S$	ΔS	ΔG
200	-114.24	40.68	203.40	-73.57	-107.60	34.95	174.75	-72.65
300	-114.15	60.93	203.10	-53.23	-103.97	48.00	160.00	-55.97
400	-113.67	80.70	201.75	-32.97	-101.18	60.78	151.95	-40.40

S3. Structure files and individual energy contributions to the *hybrid MP2:PBE+D2* values – Methanol and ethanol onto the acidic site (Al12-O20(H)) of H-ZSM5 zeolite.

VASP POSCAR files are structured as follow:

- TITLE
- Cell scaling factor
- Lattice vector parameters
- Number of each atomic species
- Coordinates (x,y,z Cartesian)

The energy contributions to the *hybrid MP2:(PBE+D2)* energies are organized as follow:

- “pbc” stands for periodic boundary conditions and “C” for cluster
- Low-level = PBE+D2
- High-level = MP2/CPC-CBS(D,T), CBS(D,T) stands for basis set extrapolation between D- and T-zeta basis set and CPC for counterpoise correction

Gas phase methanol molecule

CH3-OH

```
1.0000
20.157180    0.000000    0.000000
-0.000000   20.033350    0.000000
-0.000000   -0.000000   13.473350
```

C O H

1 1 4

Cartesian

```
10.077014233    10.017219133    6.734375703
11.499307402    10.016337504    6.704581765
 9.657876143     9.256483525    6.083690957
 9.666963534    10.984779660    6.463265574
 9.790200854     9.795166718    7.752216804
11.783266953    10.210536380    5.809219197
```

Hybrid Energy = -28.503911 eV

E_PBE+D2 (pbc) = -30.223088 eV

E_PBE+D2 (C) = -3146.455033 eV

E_MP2 (C) = -3144.735856 eV

Gas phase ethanol molecule

CH3-CH2-OH

```
1.0000
20.157180    0.000000    0.000000
-0.000000   20.033350    0.000000
```

-0.000000 -0.000000 13.473350

C O H
2 1 6

Cartesian

10.071257230	10.016837303	6.736302199
9.603222897	9.714402338	8.135330424
11.498885361	10.000031397	6.752757667
9.692233780	9.271082375	6.041603924
9.708205899	10.991437931	6.418732274
11.819574281	10.188594352	5.867379065
9.962963866	8.742186907	8.448584405
8.520215282	9.715287060	8.181381399
9.980360863	10.459040516	8.825263643

Hybrid Energy = -44.277831 eV
E_PBE+D2 (pbc) = -46.934999 eV
E_PBE+D2 (C) = -4215.250286 eV
E_MP2 (C) = -4212.593117 eV

Unloaded H-ZSM5

H-ZSM5

1.0000		
20.157180	0.000000	0.000000
-0.000000	20.033350	0.000000
-0.000000	-0.000000	13.473350

O Si Al H
192 95 1 1

Cartesian

17.967013049	19.080022283	11.671795537
18.216445087	2.991215164	11.751919965
17.968077858	14.997844247	11.673665555
18.181315947	10.879594510	11.868472327
16.314541229	17.037648043	12.183042872
19.615468766	17.041838869	12.206678997
16.297822019	4.753997271	12.307905424
16.068223676	9.303457276	12.271675574
0.443641274	2.008093126	12.273907119
0.052319185	4.664822158	12.328382507
0.368936511	12.033712206	12.247456806
0.155160085	9.361050432	12.329480005
15.818010559	11.944553252	12.365590052
8.119919551	5.262307290	12.697688394
15.816032255	2.134739755	12.425792187
7.990588797	8.902386676	12.512590914
15.537480727	19.534644780	12.599650927
15.537647447	14.559874061	12.634960597
8.034361921	0.563728062	12.839569707
12.409525381	5.426291490	12.756809248
12.026265574	0.571350118	12.844168735
12.381661918	8.631720790	12.732311691

8.018808484	13.333261562	12.838384366
12.071566342	13.435173796	12.823064284
0.124744861	14.601246857	12.899827156
0.112363329	19.474339140	12.925147863
15.395418804	7.006822014	13.333569866
0.098290140	7.011462665	0.034356812
12.490475192	2.993088455	0.263192055
12.462750738	11.035434913	0.333778445
7.575752057	11.001313718	0.606152773
7.532380569	2.966278648	0.421601048
1.897309650	0.902430963	0.708637001
1.890824250	13.101155716	0.668386119
14.471048153	4.678220970	0.783412450
1.879817890	5.146292545	0.736832823
1.916607569	8.818749916	0.780885074
14.253274685	1.056920383	0.804500286
14.269391453	12.941182075	0.806439578
14.380279944	9.256362901	0.879039316
16.888313434	13.212396408	1.006303460
16.882781977	0.789564997	1.022793089
9.302665630	4.597536480	1.546359908
19.488827716	12.691293661	1.131830630
19.482805312	1.369543745	1.128232581
6.741187508	5.300880998	1.410175097
9.434340450	9.215512946	1.258164008
16.931521408	8.676584471	1.235982167
16.937072883	5.442953486	1.325103879
9.342990354	1.357110893	1.506536719
6.838159447	8.571434255	1.351323541
9.376714649	12.703684942	1.537709300
19.525026796	4.853473574	1.438383854
19.537699127	9.189671735	1.408979016
6.761871710	0.739947739	1.664688163
6.780789191	13.280047625	1.691529888
4.321218519	9.283024727	1.798257779
4.227688091	4.735391398	1.869637643
4.171114762	1.190124342	1.971012137
11.929297276	1.014048277	1.984449741
12.093420236	5.065607655	1.906615863
4.165921746	12.930930455	1.924422676
11.953808670	8.941041748	1.880765067
11.945779605	13.080365893	1.985923926
17.763073076	11.005698872	2.209203123
2.339515332	10.999988184	2.253150744
17.713265537	3.040283732	2.156087810
2.248227355	3.014768863	2.305586186
10.225789286	7.121039840	2.689040947
5.262092943	7.012938569	2.802730536
10.170601308	19.537318359	3.236593545
10.203030576	14.668222429	3.166581753
1.934011326	0.612944241	3.338416433
2.147127859	5.434129396	3.364725592

1.908407192	13.367734574	3.312364529
18.165264834	13.408358627	3.301118147
18.180150652	0.676564998	3.317854832
2.308178651	8.615776857	3.399446163
5.407229322	19.532308454	3.578999512
5.423756096	14.555661323	3.576290118
5.870791532	2.087519496	3.800856892
18.076733943	8.759874317	3.582942118
10.388582295	2.090670441	3.831893435
18.093653276	5.200329960	3.649137542
5.755203050	11.933700143	3.785578771
5.958245012	4.746856776	3.905609301
10.397337698	12.141488943	3.933509027
9.536033243	17.081763251	3.936670141
6.105934695	9.297340036	3.799458777
10.221446063	9.503388613	3.763798433
10.343978497	4.723222672	4.100902632
6.202385908	17.051382700	4.006805859
7.864908503	19.102404059	4.467939783
8.122088060	10.942307502	4.397651839
8.129517073	3.313282811	4.402957212
7.889857687	15.022947189	4.413492777
0.184820279	9.047249176	4.937431014
0.168665530	4.957832821	5.066057081
20.141170236	0.890964579	5.143461572
20.117737132	13.168762069	5.129147030
1.845293589	7.012149149	5.447412743
18.680107119	7.020884556	5.490159202
2.066934161	14.749547712	5.533073030
2.053201352	19.294576131	5.573034237
2.378014367	1.895502175	5.623421599
18.001741880	14.708223908	5.585415204
17.765199979	12.037580666	5.517961392
18.017624015	19.399835896	5.598183036
17.802206522	2.041111786	5.543842062
10.156962714	18.880414627	5.794365364
2.323359885	12.107256885	5.621949042
10.151887863	15.263262792	5.770108997
2.653014837	4.518954938	5.833317038
2.613043474	9.492598120	5.900127446
6.125784418	3.356661992	6.130059140
5.793554556	18.649756812	6.067377688
10.112979522	3.256577905	6.184806161
5.839224023	15.441813302	6.059416010
10.146323714	10.709761926	6.089479439
6.072132765	10.598408014	6.064208865
18.026927279	9.466450578	6.152650665
17.986328268	4.603241407	6.238919674
2.808628118	17.016296007	6.631076655
18.037659529	17.049590698	6.779768617
10.506535744	13.069115956	7.230864336
5.739176283	13.003120448	7.074228793

5.726012198	0.996248655	7.222217881
10.415354138	0.952230228	7.386490167
16.264158619	10.948663650	7.411147873
16.254413309	3.049442814	7.446131952
16.239063064	18.886188612	7.506247781
16.240882157	15.221184429	7.517296570
3.886204637	2.920297252	7.534872260
3.886401691	11.130433284	7.526105052
3.751984612	19.288963868	7.645018087
3.777663675	14.734313652	7.592174573
1.262360708	3.213836428	7.686169968
1.270347727	10.841088249	7.749205410
8.670182709	19.077776517	7.973212442
8.702356298	14.878042080	7.963724789
11.298742261	18.608639880	8.131420649
18.825930712	11.366671316	7.861529845
1.239845440	15.369510146	7.987129287
18.822049687	2.686851527	7.918789633
11.306960418	15.439849231	8.099642366
1.213850550	18.626121863	8.005114790
8.749586974	2.753805182	8.335433144
18.784905534	14.871663622	8.136844193
8.775996612	11.347037733	8.243537064
18.776642126	19.213970405	8.159278596
11.376453273	10.881360638	8.406581069
11.352923771	3.148708225	8.473048874
13.830642616	19.265984712	8.534174881
13.834185984	14.773140761	8.529014470
13.955364217	2.891141435	8.649650114
13.983979993	11.111752323	8.643769893
6.145875815	18.847192814	8.690583586
6.176708393	3.123608664	8.769666870
6.165153343	15.095367350	8.667980560
6.208900496	10.928056745	8.696773968
0.447074953	0.981495634	8.871933501
15.804683698	13.047509351	8.995647068
0.391113314	13.045893914	8.946389982
15.779025512	0.976075121	9.055983994
7.906586474	16.969076075	9.413016469
12.847192104	17.014534449	9.564707757
7.912478870	4.541644174	10.135706371
7.982430720	9.396959320	9.898511466
15.859643160	18.599233006	10.119726130
0.088534519	3.361038924	10.039241674
16.230403514	10.682296492	10.055254184
16.163961963	3.366216292	10.089985779
20.135117942	10.646706924	10.039287341
15.847101365	15.435173190	10.134391506
12.682420239	4.529702280	10.262773616
12.659312879	9.477235459	10.217115218
0.077037237	15.287773882	10.323080416
0.086388548	18.834471730	10.344727164

7.999002188	19.315264014	10.552742240
12.089900399	19.315045953	10.570832382
12.423541750	1.919074232	10.581517809
7.655619376	1.931421425	10.613772852
12.436435006	12.078224097	10.554489606
7.990371353	14.609401636	10.537878095
7.719117926	11.943276739	10.616994546
12.063832212	14.710865352	10.542936848
11.959445215	7.007238658	10.720187295
8.576918070	6.994673542	10.747309485
10.039580500	0.905355924	11.079279702
10.056761002	13.051653905	11.115304828
10.270341523	9.015942211	11.178751980
10.289633092	4.992352242	11.200896973
16.419378046	18.566805740	11.642969258
19.814507084	3.264468213	11.602158457
16.625865682	3.308365665	11.644699739
16.416556021	15.504355250	11.652039428
16.581519876	10.707394672	11.637654960
19.784312342	10.727045949	11.622218428
19.523891194	15.481576634	11.769726222
19.523079739	18.604432053	11.780247558
15.640084258	0.883581956	13.453717111
15.642688603	13.152233414	13.443796997
0.412704228	13.108701997	13.468575804
0.426597102	0.927812310	13.491232033
15.764870445	5.464795700	0.202520594
15.690264908	8.564708854	0.199636077
0.343684693	5.424443171	0.263539231
0.384190415	8.591821513	0.271187747
7.962755968	4.528303639	0.667416896
12.682282590	1.421451751	0.599222148
7.977786996	9.423670278	0.572032369
12.853137473	4.552419952	0.592544902
12.688155360	12.618142884	0.617214289
12.788332253	9.464851197	0.593536548
7.912447446	1.421535280	0.741675668
7.938378476	12.573299162	0.799559607
18.072598215	12.573372155	1.909153902
18.062651378	1.472272644	1.904359058
2.721556254	9.434169339	2.057615620
2.625880546	4.578324529	2.069152286
2.570580290	1.434507276	2.086553188
2.583403484	12.595123998	2.047652073
18.080834367	9.415319027	2.100231408
18.072412527	4.626240140	2.136597754
10.444445034	8.664892915	2.403156684
5.553571466	5.449577149	2.486545539
5.632691776	8.548935804	2.433982980
10.444363928	0.979270420	2.625422118
10.468113922	13.146579763	2.656233363
5.560872850	0.887623954	2.744401536

5.547120625	13.162752158	2.740149998
9.426941434	18.640561398	4.364455813
9.445412751	15.507608012	4.329707823
6.501950714	3.370129991	4.557860442
6.316689579	18.583052784	4.533978644
6.522544379	10.697148641	4.508623098
6.337888477	15.512777606	4.516199647
9.721260043	10.808851833	4.539949480
9.696218660	3.263904218	4.646904699
1.577418100	0.668347997	4.917847519
1.706600780	5.479985242	4.925354366
1.737527811	8.545351258	4.915570041
18.516042326	13.333796170	4.883340402
1.558671771	13.343525992	4.894348566
18.537322922	0.740301617	4.899095868
18.783139119	8.574055080	5.032225206
18.771276429	5.449530670	5.100008994
2.526379196	3.129828311	6.674568140
2.507575093	10.903454973	6.703103122
17.737760034	10.953369944	6.730876789
17.735190192	3.094844453	6.782801451
2.471715018	15.460429176	6.940050357
2.457066039	18.561710876	6.968148469
17.769848959	15.464864073	7.006571294
17.772170278	18.632935364	7.011875027
10.130467932	19.385594705	7.330555984
10.159230628	14.652391901	7.270882213
5.469132312	2.591322229	7.409815534
5.352638690	19.458516078	7.405261450
5.473438895	11.417769968	7.335688244
5.377377842	14.562533096	7.346406341
10.209158238	11.490323439	7.492146371
10.158964289	2.515098739	7.623080718
0.117294719	2.555547510	8.627600543
0.080578129	11.478809204	8.646744251
15.427217705	19.444849455	8.802799619
15.563386934	11.452522280	8.786128476
15.537959949	2.566724789	8.819891796
15.432527876	14.614145588	8.795136837
0.077032640	14.635816699	8.840149288
0.083247322	19.430680875	8.839742418
7.679612823	18.549682329	9.157636691
12.519795202	18.558471513	9.198956437
7.697075894	15.385273436	9.142799937
12.513626308	15.473452652	9.180982019
7.637355508	3.090901227	9.477634253
7.688574799	10.902504617	9.365709356
12.591807075	3.122448033	9.497232329
12.595203684	10.888326133	9.450827477
8.724640981	5.446631208	11.211840905
8.705549466	8.573422756	11.097030750
8.439060100	0.668423108	11.273234441

11.638896350	0.674068703	11.272939855
11.827455312	8.531826244	11.211222461
11.844933192	5.490466967	11.241677382
8.449287122	13.237554459	11.277457827
11.652265710	13.314132933	11.260800450
10.503936663	5.472043852	2.381488741
10.738115272	5.253868206	4.802830850

Hybrid Energy = -2234.972910 eV
E_PBE+D2 (pbc) = -2303.956624 eV
E_PBE+D2 (C) = -118755.460497 eV
E_MP2 (C) = -118686.476782 eV

Adsorption complex: Methanol/H-ZSM5

CH3-OH/H-ZSM5

1.0000		
20.157000	0.000000	0.000000
-0.000000	20.033000	0.000000
-0.000000	-0.000000	13.473000

O	Si	Al	H	C
193	95	1	5	1

Cartesian

9.352481384	8.172356726	11.400813113
9.324468839	12.151133632	11.298499670
9.123210921	16.283603348	11.198085095
9.121361471	4.029727642	11.189543082
7.621701258	10.136142057	10.862698538
11.030491320	10.156777012	10.841221541
11.191535701	17.881748173	10.686812507
6.781497987	15.172299159	10.745166415
7.036878960	17.842320916	10.676859947
11.486314320	15.240852436	10.686607641
6.778442134	5.156696775	10.747543866
11.493881426	5.065819193	10.685300383
11.187548384	2.425873583	10.674943818
7.016948698	2.484309568	10.699747623
19.333410678	1.930317251	10.454411337
19.315391715	18.420374201	10.444318564
11.710978311	12.637312257	10.362524096
11.700357499	7.680908644	10.344874930
14.917258791	18.577092181	10.243830792
19.214691158	13.801955550	10.161414674
15.232870372	6.507180090	10.197996590
15.307214125	13.828265454	10.192817167
19.298567559	6.515650593	10.144296279
14.918539484	1.717250301	10.217965725
6.984800355	12.582350496	10.160084205
7.123889066	7.707830539	10.040862793
11.926759870	0.129643258	9.639187904
7.007418659	0.154176921	9.498450086

14.840637591	4.128273556	9.148508861
19.631083385	16.193207007	9.044585472
14.884989241	16.188536243	9.115336652
19.666240691	4.127499466	9.001737936
5.266787182	14.084246283	8.868879234
5.222702478	18.332574570	8.793353757
5.283523304	6.244023977	8.842392751
5.217869715	2.014026730	8.800179615
13.056860081	14.257332174	8.794031351
13.018979249	6.053476886	8.757707978
12.910513191	17.906502330	8.632029717
12.902293670	2.380867141	8.614945766
10.407576788	6.264361238	8.565646284
10.457666149	14.044940923	8.526321469
17.856602032	2.314756912	8.275278301
7.847832534	14.427760632	8.418995497
17.853203471	18.017351231	8.264148283
7.827714868	5.747863451	8.376483726
0.299374726	1.754192807	8.111541736
10.371084264	18.530673527	8.240834691
17.890592841	5.822139917	8.019301429
0.303142268	18.533475617	8.102724041
17.901594078	14.503020810	7.984330443
10.358742999	1.735759875	8.247903891
7.753639468	18.038692616	8.106170018
7.756196401	2.327035487	8.140275308
0.350141855	13.979645356	7.868789846
0.334025532	6.347844495	7.800589627
2.843208847	17.905523754	7.719415680
2.833444895	2.406070596	7.717291868
2.967618655	14.279640783	7.648901271
2.961398021	6.062162964	7.657743332
15.315329286	18.357398854	7.626047175
15.320627944	2.003924666	7.607239483
15.322310645	6.211990184	7.554666631
15.334615184	14.078151481	7.547495174
9.567221002	4.095076899	7.329714845
4.794136637	4.149925669	7.257904103
4.818439073	16.178349050	7.276109269
9.494744085	16.198183279	7.325083677
17.111421228	0.156139749	6.892277736
1.867857100	0.134653393	6.721828045
17.070317830	7.738060290	6.334177496
17.092309567	12.600190469	6.282669665
5.196846131	13.797432451	6.234035821
9.191535842	13.808536986	6.244297635
4.908048987	18.577843567	6.172999094
9.194024254	6.467707400	6.272329572
4.907956642	1.733338026	6.187736759
5.157256044	6.534541975	6.202059263
1.700318618	12.629749802	6.025109733
1.726117013	7.661979084	5.957902925

9.196052170	18.438593972	5.914106144
1.408448694	15.242875642	5.740182972
9.160332868	1.872087468	5.940700017
16.852225069	5.172818995	5.654881412
17.114415761	2.503279451	5.707992198
16.827587847	15.174195103	5.648838196
17.087895576	17.843474419	5.707238596
1.458333213	5.039892898	5.735420336
1.107964512	2.410222088	5.665789787
1.132125475	17.883811607	5.659620733
17.759736628	10.160072300	5.604724525
9.241389413	9.917635631	5.674414655
0.921940561	10.150306080	5.565038551
19.191554303	16.285237456	5.261698447
19.211605607	4.064962885	5.252912108
19.407193083	8.102166789	5.151984143
19.419413902	12.196157787	5.087747695
6.955628209	18.182021261	4.521429273
7.201058512	6.327992078	4.525072463
7.201561733	13.956894751	4.494589734
6.931924491	2.169804302	4.521755795
5.233630853	0.147847125	4.105466564
9.266002748	7.945483277	4.143443264
9.325408261	12.490171898	4.004701177
5.067254792	12.428370671	4.013446640
8.641155281	0.170909808	3.994065899
9.480056507	15.152503026	4.017343876
5.129872034	7.891153852	3.953698263
4.883472564	15.075760765	3.915109546
17.168810940	8.357811264	3.748440974
9.538989679	5.320979734	3.924148667
17.164469000	11.917685121	3.711213974
4.887943327	5.242427433	3.886602535
4.489089816	17.679988715	3.696375794
4.449280971	2.642528617	3.723788782
1.362715790	11.758297457	3.522214427
17.255902266	3.816862778	3.426720218
17.244760066	16.536274966	3.428482450
0.975228578	16.507699977	3.438779822
1.260190469	8.570295463	3.482479114
0.993515462	3.774605293	3.438705252
9.284330282	17.729171520	3.353670730
9.273831226	2.693834432	3.426432908
4.333365831	10.160193694	2.916451676
9.284346427	10.267471150	2.678656186
1.353150040	6.160653348	2.395497821
16.789352622	6.184488124	2.274291209
1.372354199	14.137072400	2.368543797
16.828138076	14.146490300	2.313468632
11.008398695	16.179104379	2.112880162
11.027582730	12.155715070	2.027991256
3.235696361	16.027235779	2.068939545

11.154160253	8.188376223	2.008335252
10.999987989	4.143892325	2.083563857
3.236175298	4.288938810	2.054296877
3.334040383	7.879788942	1.970890824
3.377187175	12.436662726	1.931110408
5.835004215	16.418780041	1.790919604
5.833580405	3.825395476	1.802143341
18.601400247	12.325878381	1.518466982
18.620426007	7.981108280	1.555186140
8.426056010	15.831809737	1.673080142
5.926325715	11.815336757	1.580096549
8.399276801	4.509947834	1.674729390
16.038994146	8.583767589	1.407741002
15.992174962	11.806178987	1.381557687
8.499623944	12.524651474	1.489958759
5.830655882	8.537794830	1.454994178
18.555586561	4.520098665	1.236028889
18.557024477	15.836021718	1.248188267
8.399895021	7.811027224	1.441062667
15.961516479	3.933248154	1.130738733
15.953365163	16.367585627	1.140457028
13.447904619	12.396879097	0.996641425
13.331013698	16.110516021	0.921502555
13.333181280	4.183079957	0.920443296
0.983072909	11.951050944	0.899495621
0.974308071	8.307111079	0.854989884
13.556884699	7.819771735	0.934110503
0.964946475	16.256305109	0.797956412
0.961617264	4.049954395	0.803466368
6.520997741	6.107563404	0.658161032
6.643974040	14.183685571	0.607186784
11.556896553	14.187076580	0.407955730
11.588883160	6.125967031	0.364546308
19.324761929	10.146784140	0.147470882
14.461760708	10.149495285	13.457209919
19.327450445	2.580787104	13.036264302
19.351284164	17.744563479	13.020095104
11.110043963	16.594055446	12.957840639
7.123464358	16.560630729	12.967572433
11.418759730	11.763257431	12.877396292
11.114690684	3.707297681	12.947456477
11.545302488	8.559333599	12.856188870
7.123524017	3.772194409	12.973298707
14.615847346	17.708230467	12.749130994
14.620957036	2.646031263	12.702479167
7.121583538	11.935833158	12.747713619
14.887397628	5.278757363	12.538354254
7.016281332	8.243787120	12.643313968
14.892867340	15.088000991	12.503533976
19.385257641	12.500756571	12.443607957
19.615529218	15.174160627	12.375336923
19.307766550	7.799999101	12.445131114

19.653727422	5.139720538	12.365329909
15.159585599	12.448811177	12.409662295
15.332326094	7.902273275	12.407220884
18.681908997	0.149331367	12.318255713
15.391828944	0.151914835	12.280472302
17.263341195	14.037077371	11.996384993
17.041349797	18.136496492	11.781001240
17.280433605	6.165441498	11.874681809
17.042166715	2.188039296	11.749630485
10.722297922	16.494810368	11.385751797
7.518599487	16.467392317	11.396566515
10.915854045	8.638144299	11.369839402
10.883661896	11.675527013	11.346545978
10.721821702	3.813215167	11.379458527
7.515338455	3.861210681	11.404942782
7.760349947	11.697403650	11.277570218
7.778584151	8.566171647	11.257905609
11.660762460	14.047557669	9.591412011
11.643304119	6.264166179	9.593147192
6.739466117	14.066857858	9.552542564
6.762033396	6.218032080	9.515214997
11.598797722	18.613982448	9.294481305
6.758838315	18.602764581	9.268116749
11.596124982	1.677209279	9.292969639
6.750827147	1.739485204	9.282675018
19.319912874	2.540512957	8.954348624
19.308275033	17.782845007	8.955855622
14.508431426	17.753274916	8.905224969
14.600492978	5.720741175	8.923282748
14.639533429	14.593118760	8.921683471
14.496474432	2.562393312	8.896223914
19.317008063	14.623507254	8.762616101
19.338568068	5.698702545	8.739000723
9.251988379	5.636427494	7.654577800
9.254857548	14.619666059	7.634741742
4.445530874	17.744147471	7.488240641
4.554060893	14.589141074	7.501335505
4.434924068	2.582570268	7.489651723
4.544353744	5.742027853	7.485892948
9.199806805	17.794484147	7.401286585
9.204133302	2.510805332	7.424422473
16.854937593	1.741829301	7.121870426
16.846397743	18.605641617	7.123696570
1.528249137	1.683388072	7.058691951
1.535298290	18.616808044	7.055179751
16.801948711	6.235925866	6.886900299
16.806734010	14.087852681	6.860876864
1.590415034	14.042342485	6.825586972
1.602784146	6.269588049	6.793706474
17.852339035	8.591721201	5.199563270
17.861270340	11.717347372	5.162479322
17.610419288	3.885990035	5.008475286

0.630450976	16.476366157	5.021661468
17.591289497	16.462477354	5.011266248
0.812397383	11.686364397	5.045741570
0.792371481	8.619268482	5.034870869
0.645522982	3.826674234	5.019743164
8.778272145	6.472336215	4.727256462
8.795001254	13.858526140	4.684844961
5.397088162	18.651169940	4.627844198
5.590540558	13.820662197	4.663284060
5.380759908	1.676032206	4.636720202
5.584189595	6.495737255	4.639619122
8.518751707	18.645143747	4.451882368
8.499452076	1.722669607	4.467235464
4.623187203	16.288734702	2.862753160
4.614842488	4.011828516	2.857516768
9.533844385	16.226066511	2.790730828
9.534665463	4.157439693	2.771412651
4.675865268	11.711956348	2.603439955
4.663197031	8.610116085	2.564602929
9.524901057	11.820045846	2.525474707
17.158749590	7.767884633	2.240880722
17.151934839	12.556109608	2.222304819
1.644740534	15.728966912	2.175862732
1.644343513	4.574424059	2.179410564
1.732213032	7.725319329	2.176202846
1.774075715	12.575068096	2.179694033
17.137369633	4.617010220	2.015595864
17.143017104	15.715814408	2.029032780
7.006611480	15.743511444	0.894382145
6.970220975	4.570018168	0.908105947
11.860385367	12.621610336	0.712881563
11.754809900	15.766016654	0.731011737
11.941005181	7.684115379	0.709986481
7.057022446	12.614898085	0.742868177
11.763616835	4.554277615	0.708653824
6.989642194	7.677328017	0.698027391
19.608817418	11.726731302	0.384551953
19.591427708	8.562344207	0.380561824
14.764018518	11.702866771	0.329622502
14.835079958	8.605339449	0.318918008
19.646169416	4.070627518	0.119300208
19.645441375	16.255044388	0.118967905
14.714250835	16.307013308	0.096041320
14.717078979	4.024196726	0.090465191
18.595616945	1.710214249	11.883009704
18.596438371	18.621496657	11.885187535
18.865449901	13.874608765	11.744958767
15.663417064	13.855628495	11.774337116
15.491770689	18.649093403	11.759533619
15.686141352	6.458221523	11.754883598
18.880981562	6.413323131	11.710714077
15.492487288	1.680461282	11.736073317

9.547673952	8.593596367	2.435389528
9.766019450	10.886497537	7.428913708
10.028354830	9.140336737	7.378415515
11.129011538	10.217698775	6.512061558
9.262375152	10.729103794	5.145156441
9.284582541	8.734490818	4.823083673
10.102320748	10.060056230	6.817143470

Energy (total) = -2264.501154 eV
 E_PBE+D2 (pbc) = -2335.393209 eV
 E_PBE+D2 (C) = -121903.112318 eV
 E_MP2 (C) = -121832.220263 eV

Adsorption complex: Ethanol/H-ZSM5

CH3-CH2-OH/H-ZSM5

1.0000		
20.157180	0.000000	0.000000
0.000000	20.033350	0.000000
0.000000	0.000000	13.473350

O	Si	Al	H	C
193	95	1	7	2

Cartesian

17.930856356	2.190567089	11.534223835
18.162987247	6.183204529	11.660746675
17.931349199	18.141945333	11.561958456
18.147211634	14.026436746	11.779028811
16.278825284	0.154791885	12.061016325
19.571482697	0.153087448	12.105355504
16.208037904	7.909510151	12.199983556
16.037128400	12.446988401	12.192729100
0.371844941	5.144128554	12.156044537
0.040198053	7.806731453	12.235095106
0.334048012	15.179208794	12.159792284
0.121564122	12.504526987	12.228085731
15.780604096	15.087374515	12.284173670
7.881573283	8.256173250	12.414800358
15.774575083	5.282843677	12.322470455
7.981780269	11.943659297	12.513056245
15.510146947	2.649152107	12.487293583
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9.926592768	10.735247024	4.925169484
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12.186007244	9.515182152	6.477413523
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10.132825311	10.050527354	6.791484048
11.609300044	10.315291113	6.926930828

Hybrid Energy = -2280.401533 eV
 E_PBE+D2 (pbc) = -2352.266541 eV
 E_PBE+D2 (C) = -122972.004202 eV
 E_MP2 (C) = -122900.139193 eV

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2. Alexopoulos, K.; Lee, M.-S.; Liu, Y.; Zhi, Y.; Liu, Y.; Reyniers, M.-F.; Marin, G. B.; Glezakou, V.-A.; Rousseau, R.; Lercher, J. A., Anharmonicity and Confinement in Zeolites: Structure, Spectroscopy, and Adsorption Free Energy of Ethanol in H-ZSM-5. *J. Phys. Chem. C* **2016**, *120* (13), 7172-7182.