Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Activation of CO_2 and CH_4 on MgO Surfaces: Mechanistic Insights from First-Principles Theory

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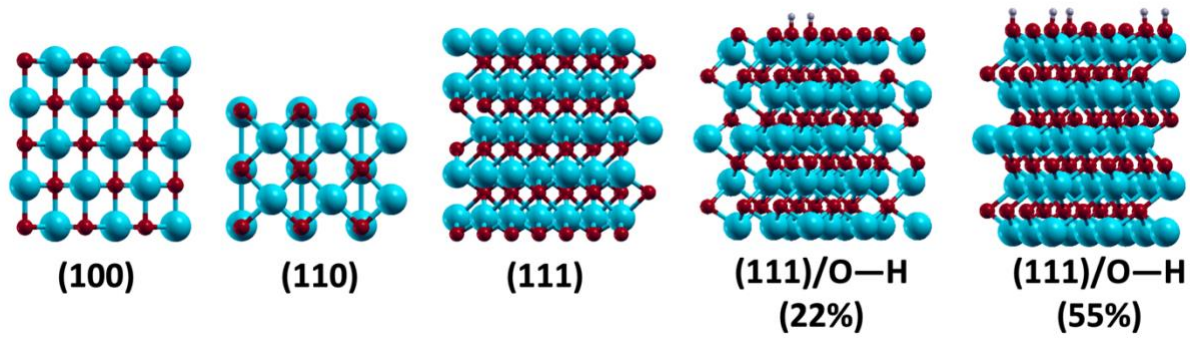

Figure S1. Optimized structures of various surfaces of MgO investigated in this work. Blue, red and gray atoms indicate Mg, O and H, respectively.

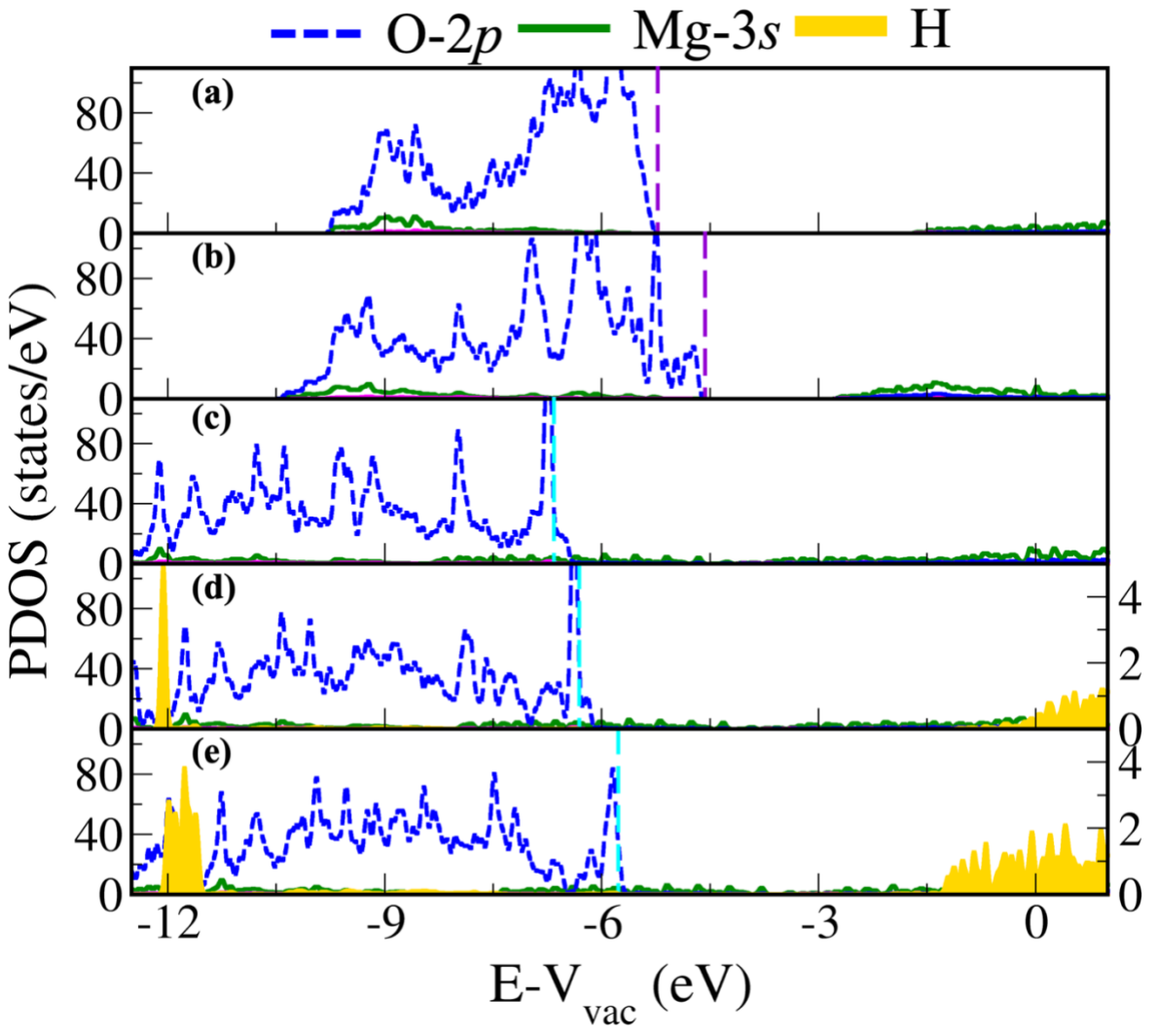

Figure S2. Projected density of states (PDOS) of the (a) (100), (b) (110), (c) (111), (d) (111)/O—H (22% hydroxylation), and (e) (111)/O—H (55% hydroxylation) surfaces of MgO. Alternate *y*-axis represents the DOS of H atoms. The energies are with respect to vacuum potential. Dashed purple and blue lines represent the VBM and Fermi level, respectively.

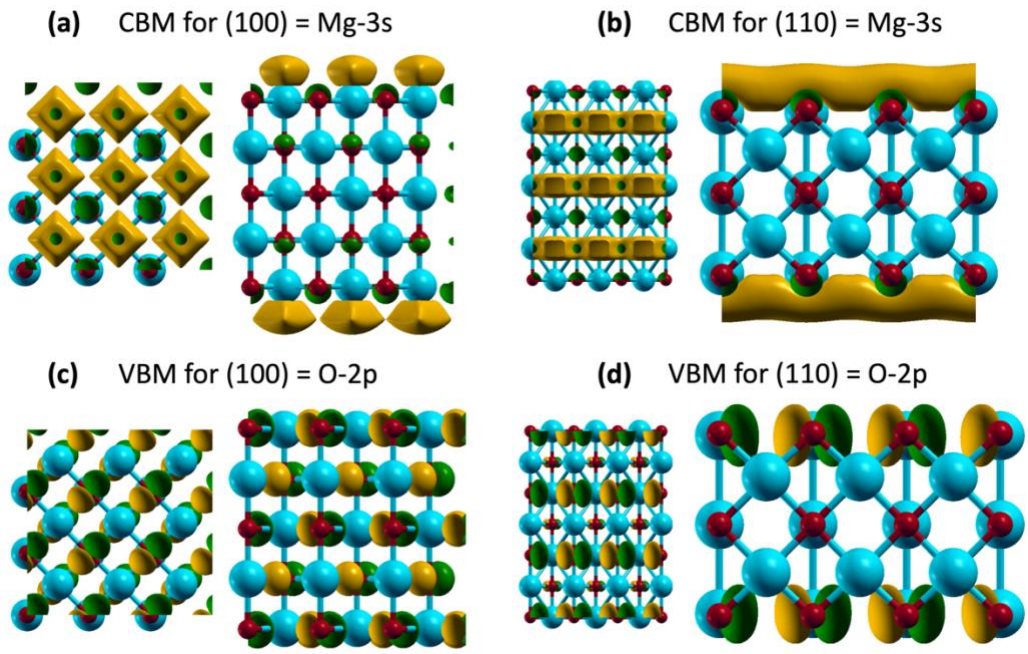

Figure S3. Isosurfaces for the conduction band maximum (CBM) of the (a) (100) surface, (b) (110) surface, and valence band minimum (VBM) for the (c) (100) surface and (d) (110) surface. Green and yellow in the isosurfaces correspond to positive and negative sides, respectively. For each subfigure, the isosurface on the left proves the *xy* view and the isosurface on the right provides the *xz* view (note that the vacuum is along the *z*-axis).

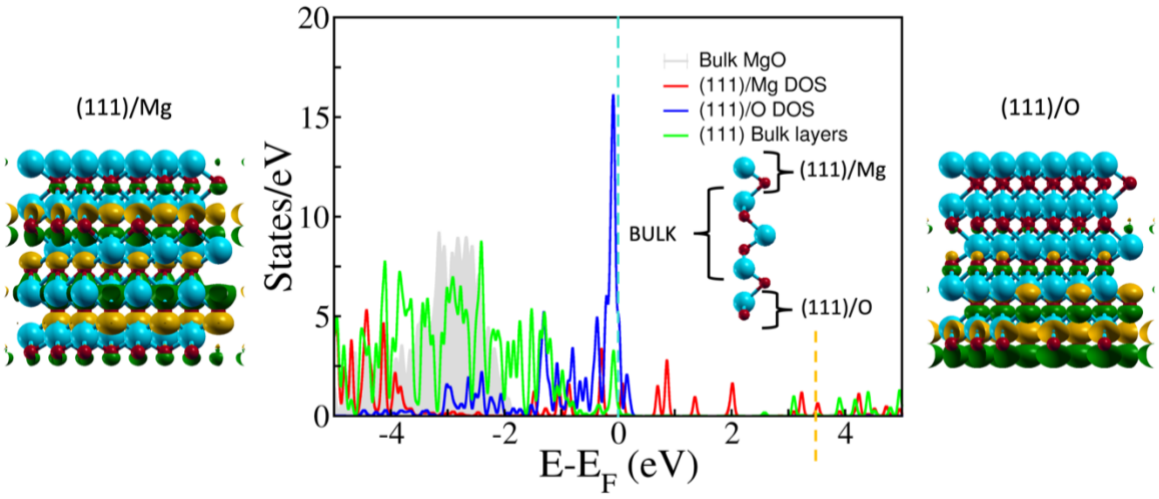

Figure S4. Locally resolved density of states (LDOS) of the (111) surface of MgO. The inset figure shows the planes whose states are represented by the red (O-terminated), blue (Mg-terminated) and green (bulk) curves. The isosurfaces of the Mg-terminated, (111)/Mg, and O-terminated, (111)/O planes of the surface are shown alongside. Green and yellow in the isosurfaces correspond to positive and negative sides, respectively. The shaded gray region are the states of bulk MgO and the vertical orange dashed line indicates the energy where the CBM of bulk MgO begins. The energies are plotted with respect to the Fermi energy and the dashed blue line represents the Fermi level.

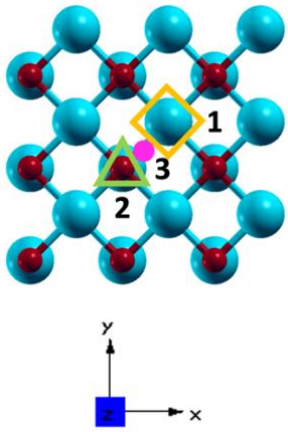

Figure S5. Sites on MgO surface which are considered for adsorption studies. Mg and O atoms are denoted by blue and red, respectively. For representative purposes, the (100) surface of MgO is shown here. Site 1, above Mg, represented as an orange rhombus, Site 2, above O, represented as a green triangle, and Site 3, above the bond connecting Mg and O, shown as a filled magenta circle.

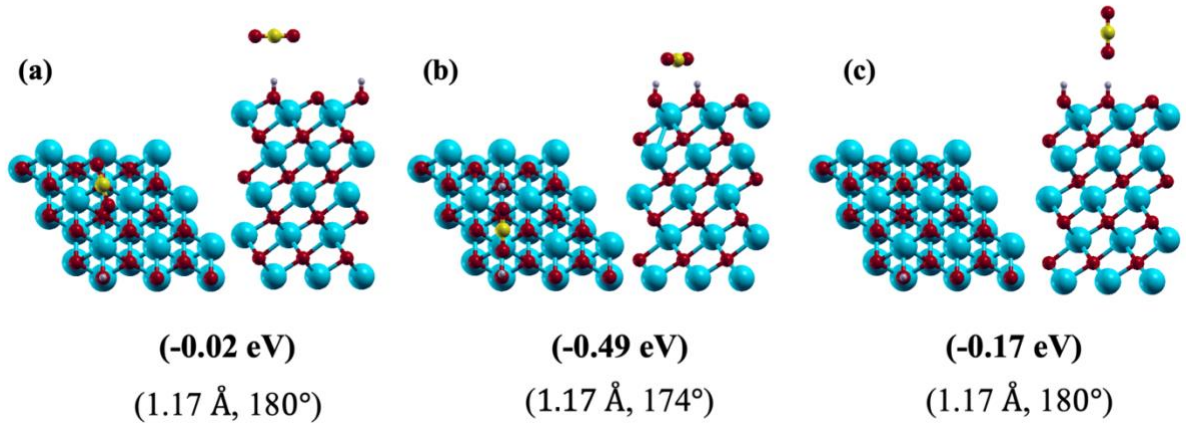

Figure S6. Optimized structures of CO_2 adsorbed on 22% (111)/O—H surface of MgO. See Table S4 for the initial geometries for these optimized structures. The bold numbers indicate adsorption energies, and those below indicate the bond lengths and angle in CO_2 following adsorption.

Reaction equations for the cases with high adsorption energies

$$\mathrm{MgO\ (111)/O} + H_2 \rightarrow 2H^* + \mathrm{MgO(111)/O} \qquad \Delta\mathrm{H} = -7.88\ \mathrm{eV}$$

$$\mathrm{MgO\ (111)/O} + \frac{5}{2}H_2 \rightarrow 5H^* + \mathrm{MgO(111)/O} \qquad \Delta\mathrm{H} = -18.99\ \mathrm{eV}$$

$$\mathrm{MgO\ (111)/O} + CH_4 \rightarrow H^* + CH_3^* + \mathrm{MgO(111)/O} \qquad \Delta\mathrm{H} = -6.82\ \mathrm{eV}$$

$$\mathrm{MgO\ (111)/O} + CH_4 \rightarrow 3H^* + CH^*(\mathrm{bidentate}) + \mathrm{MgO(111)/O} \qquad \Delta\mathrm{H} = -17.91\ \mathrm{eV}$$

Negative enthalpies indicate energy released. * indicates an entity adsorbed on surface. Reference energies of adsorbates are E_{H_2} or E_{CH_4} which account for energy of cleavage of bonds in the source molecules.

Table S1. CO_2 adsorption energies, and CO_2 adsorption energies without dispersion correction for the various pristine surfaces studied in this work. All values are given in eV. Highlighted structures correspond to those, whose electronic structure is shown in Figure 2 of the main paper.

Surface	Initial adsorption site	ΔE_{ads}	$\Delta E_{ads}^{\dagger}$
(100)	Site 1	-0.119	0.037
	Site 2	-0.599	-0.318
	Site 3	-1.004	-0.739
(110)	Site 1	-0.025	0.023
	Site 2	-3.264	-2.973
	Site 3	-2.393	-2.133
(111)/Mg	Site 1	-0.123	-0.023
	Site 2	-2.137	-1.854
	Site 3	-0.129	-0.025
(111)/O	Site 1	-0.221	0.000
	Site 2	-0.188	-0.020
	Site 3	-0.198	-0.002

Table S2. Calculated Lowdin charges on C and O atoms of CO_2 in free form and in MgO-CO_2 adsorbed complexes (first row of the table gives Lowdin charges for an isolated CO_2 molecule). The highlighted charges correspond to adsorbed complexes in which CO_2 molecule is activated and chemisorbed on MgO.

Adsorbed complex	Atom	Number of valence electrons		Total number of valence electrons	Lowdin charge on CO_2 molecule
		s	p		
Isolated CO_2 molecule	C	0.74	3.18	16.24	-0.24
	O	1.66	4.50		
	O	1.66	4.50		
(100) at Site 1	C	0.74	2.49	15.76	0.24
	O	1.66	4.61		
	O	1.66	4.61		
(100) at Site 2	C	0.82	2.57	16.42	-0.42
	O	1.69	4.83		
	O	1.69	4.83		

(100) at Site 3	C	0.82	2.57	16.45	-0.45
	O	1.69	4.85		
	O	1.69	4.85		
(110) at Site 1	C	0.74	2.47	15.75	0.25
	O	1.66	4.61		
	O	1.66	4.61		
(110) at Site 2	C	0.80	2.49	16.48	-0.48
	O	1.69	4.91		
	O	1.69	4.91		
(110) at Site 3	C	0.81	2.52	16.62	-0.62
	O	1.69	4.96		
	O	1.69	4.96		
(111)/Mg at Site 1	C	0.75	2.48	15.77	0.23
	O	1.66	4.61		
	O	1.66	4.61		
(111)/Mg at Site 2	C	1.27	2.68	17.22	-1.22
	O	1.71	4.92		
	O	1.71	4.92		
(111)/Mg at Site 3	C	0.75	2.48	15.77	0.23
	O	1.66	4.61		
	O	1.66	4.61		
(111)/O at Site 1	C	0.74	2.46	15.61	0.39
	O	1.66	4.54		
	O	1.66	4.54		
(111)/O at Site 2	C	0.74	2.22	15.49	0.51
	O	1.66	4.62		
	O	1.66	4.59		
(111)/O at Site 3	C	0.74	2.34	15.10	0.90
	O	1.67	4.36		
	O	1.66	4.34		

Table S3. CH_4 adsorption energies, and CH_4 adsorption energies without dispersion correction for the various pristine surfaces studied in this work. All values are given in eV. Highlighted structures correspond to those, whose electronic structure is shown in Figure 5 of the main paper.

Surface	Initial adsorption site	ΔE_{ads}	$\Delta E_{ads}^{\dagger}$
(100)	Site 1	-0.302	-0.064
	Site 2	-0.123	0.022
(110)	Site 1	-0.415	-0.160
	Site 2	-0.142	0.005
(111)/Mg	Site 1	-0.114	-0.008
	Site 2	-0.097	-0.019
(111)/O	Site 1	-17.910	-17.551
	Site 2	-6.816	-6.756

Table S4. Energies (in eV) correlated with number of interactions of O atoms on (111)/O surface of MgO.

Surface	Stabilization energy/ Adsorption energy (eV)	Number of interactions of O atoms	Type of interactions of surface O atoms	Energy scaled by number of interactions of O atoms (eV)
22% (111)/O—H	-7.88	2	2 O—H bonds	-3.94
55% (111)/O—H	-18.99	5	5 O—H bonds	-3.80
CH_4 adsorbed on (111)/O (cleavage of 1 C—H bond)	-6.82	2	1 O—H bond 1 O—CH_3 bond	-3.41
CH_4 adsorbed on (111)/O (cleavage of 3 C—H bonds)	-17.91	5	3 O—H bonds 2 O—CH bonds	-3.58

Table S5. Adsorption energies, and adsorption energies without dispersion correction of CO_2 and CH_4 for the hydroxylated surfaces studied in this work. All values are given in eV. Highlighted structures correspond to those, whose electronic structure is shown in Figure 7 of the main paper.

Adsorbate	Surface	Initial adsorption site	ΔE_{ads}	$\Delta E_{ads}^{\dagger}$
CO_2	22% (111)/O—H	Site 2	-3.398	-3.096
		(a) C of CO_2 above H	-0.016	0.063
		(b) O of CO_2 above H	-0.491	-0.279
		(c) CO_2 vertically above H	-0.166	-0.115
	55% (111)/O—H	Site 2	-3.218	-2.887
CH_4	22% (111)/O—H	Site 2	-6.501	-6.068
	55% (111)/O—H	Site 2	-0.138	0.008

Cartesian coordinates for some relevant geometries

All values are given in Angstroms, and '0 0 0' indicate frozen coordinates.

Optimized structure – 22% (111)/O—H surface

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Optimized structure – 55% (111)/O—H surface

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O 2.402748140 6.069825414 2.486378421
Mg 3.904204630 5.201819951 1.399895911

Structure – (111)/O—CH_4^{Str1}

CELL_PARAMETERS {alat=9.013}

1.000000000000d0 0.000000000000d0 0.000000000000d0
-0.500001664841d0 0.866026923807d0 0.000000000000d0
0.000000000000d0 0.000000000000d0 2.885724333438d0

Starting geometry of (111)/O—CH_4^{Str1}

C 2.402661 4.334890 14.098442
O 2.402623 2.600927 11.948442
Mg 0.900833 1.733811 11.067295
O -0.600949 2.600743 11.948254
Mg -0.600749 4.334741 11.067273
O -2.102599 5.201698 11.948220
Mg -2.102763 6.936039 11.067397
Mg 3.904355 1.733861 11.067329
O 5.405960 2.600948 11.948345
Mg 6.908054 1.734057 11.067516
O 6.907882 -0.000157 11.948146
Mg 2.402661 4.334890 11.067307
O 3.904302 5.201909 11.948299
Mg 3.904318 6.936320 11.067619
O 3.904553 -0.000181 11.948245
O 0.900976 5.201881 11.948392
Mg 0.900733 6.936092 11.067464
O 0.900970 -0.000361 11.948064
Mg 5.406317 4.335066 11.067464

O	-0.600683	6.069137	9.659880	
Mg	0.900977	5.201977	8.639892	
O	2.402688	6.069170	9.659902	
Mg	3.904547	5.202125	8.639882	
O	3.904367	3.467922	9.659877	
Mg	5.406229	2.601087	8.639927	
O	5.406046	0.866878	9.659818	
Mg	6.907938	-0.000258	8.639991	
Mg	-2.102495	5.201910	8.639977	
O	-3.604308	6.069015	9.659852	
O	-2.102622	3.467763	9.659833	
Mg	-0.600823	2.600874	8.640045	
O	0.900989	3.467889	9.659861	
Mg	2.402631	2.600953	8.639933	
O	2.402668	0.866848	9.659798	
Mg	3.904349	-0.000395	8.639979	
O	-0.600953	0.866728	9.659776	
Mg	0.900869	-0.000457	8.640083	
O	5.406271	4.334824	7.275807	
Mg	3.904401	3.467957	6.240769	
O	2.402597	4.334832	7.275908	
Mg	2.402722	6.069085	6.240884	
O	3.904556	6.936138	7.275754	
O	3.904268	1.733842	7.275938	
Mg	2.402680	0.866633	6.240702	
O	0.900915	1.733828	7.275934	
Mg	-0.600997	0.866634	6.240831	
Mg	5.406083	0.866672	6.240740	
O	6.907941	1.733834	7.275840	
Mg	0.901003	3.467913	6.240733	
O	-0.600755	4.334818	7.275903	
Mg	-2.102673	3.467913	6.240858	
O	0.900884	6.936144	7.275854	
Mg	-0.600675	6.069043	6.240844	
O	-2.102469	6.936130	7.275848	
Mg	-3.604356	6.069045	6.240973	
O	2.402623	2.600975	4.879260	0 0 0
Mg	0.900878	1.733758	3.841750	0 0 0
O	-0.600924	2.600863	4.879265	0 0 0
Mg	-0.600791	4.334803	3.841724	0 0 0
O	-2.102595	5.201843	4.879235	0 0 0
Mg	-2.102631	6.936104	3.841859	0 0 0
Mg	3.904276	1.733799	3.841785	0 0 0
O	5.406035	2.601007	4.879159	0 0 0
Mg	6.907937	1.733940	3.841856	0 0 0
O	6.907882	-0.000250	4.879037	0 0 0
Mg	2.402608	4.334844	3.841761	0 0 0
O	3.904364	5.201988	4.879131	0 0 0
Mg	3.904427	6.936284	3.841965	0 0 0
O	3.904470	-0.000282	4.879136	0 0 0
O	0.900954	5.201956	4.879230	0 0 0
Mg	0.900768	6.936143	3.841896	0 0 0
O	0.900922	-0.000394	4.879140	0 0 0
Mg	5.406267	4.334985	3.841828	0 0 0
O	0.900998	3.467942	2.480698	0 0 0
Mg	-0.600804	2.600880	1.401124	0 0 0
O	-2.102631	3.467797	2.480596	0 0 0
Mg	-2.102476	5.201910	1.401120	0 0 0
O	-3.604312	6.068961	2.480542	0 0 0
Mg	2.402597	2.600928	1.401025	0 0 0

O	3.904352	3.467957	2.480721	0 0 0
Mg	5.406136	2.601028	1.401090	0 0 0
O	5.406038	0.866913	2.480654	0 0 0
Mg	6.907841	-0.000119	1.401206	0 0 0
Mg	0.900926	5.201959	1.401021	0 0 0
O	2.402671	6.069120	2.480668	0 0 0
Mg	3.904465	5.202059	1.401086	0 0 0
O	2.402683	0.866897	2.480632	0 0 0
Mg	0.900902	-0.000266	1.401241	0 0 0
O	-0.600945	0.866753	2.480529	0 0 0
Mg	3.904302	-0.000220	1.401142	0 0 0
O	-0.600683	6.069104	2.480645	0 0 0
H	2.402651	3.896577	15.095339	
H	2.402685	5.420877	14.179389	
H	3.291819	4.011033	13.559520	
H	1.513489	4.011072	13.559520	

Final geometry of (111)/O—CH_4^{Str1}

C	2.407354620	6.060103304	12.564627154
O	2.401872176	2.612119076	11.950754727
Mg	0.891188151	1.721424495	11.048714724
O	-0.560471668	2.565342562	11.960350586
Mg	-0.587501236	4.339183797	11.250036034
O	-2.110890392	5.248982161	11.965369846
Mg	-2.102630301	6.917719606	11.032860665
Mg	3.911935941	1.726191929	11.045419403
O	5.361695450	2.562700123	11.968712090
Mg	6.905546281	1.630951326	11.348352009
O	6.913695404	-0.403393458	12.064173296
Mg	2.396356920	4.276060566	10.872440797
O	3.567180587	5.390362213	12.067946234
Mg	3.947137636	6.943698502	10.859157539
O	3.927496912	-0.027369600	11.947110918
O	1.249808288	5.393966858	12.078334697
Mg	0.857281755	6.941471307	10.869431842
O	0.877153598	-0.031817295	11.945412480
Mg	5.350023336	4.352725546	11.303571643
O	-0.575129397	6.077101529	9.677301135
Mg	0.882566569	5.181080581	8.585018101
O	2.401377511	6.056381825	9.572484786
Mg	3.920849541	5.177797817	8.586152815
O	3.871995335	3.469063587	9.681187780
Mg	5.429113139	2.600127902	8.726192170
O	5.403763568	0.819676627	9.683795557
Mg	6.909371490	0.009214474	8.592242392
Mg	-2.105288383	5.182339412	8.698962402
O	-3.633959470	6.079413652	9.670308663
O	-2.094085880	3.475083307	9.685899127
Mg	-0.616960476	2.594746386	8.716574542
O	0.928401657	3.471591967	9.678186735
Mg	2.402159080	2.572677332	8.596066502
O	2.403125988	0.855092059	9.697948560
Mg	3.892848228	0.000080022	8.593766063
O	-0.594198090	0.818251823	9.680456477
Mg	0.915838069	-0.001098881	8.592650847
O	5.400012536	4.331927977	7.283985111
Mg	3.911657725	3.454100644	6.232556772
O	2.402092772	4.315170270	7.255793177

Mg	2.401048003	6.063753118	6.227248811			
O	3.912069063	6.935543415	7.254966725			
O	3.897265177	1.720431762	7.285913663			
Mg	2.402906909	0.860479045	6.215375751			
O	0.907840187	1.722128168	7.287023660			
Mg	-0.600389291	0.869401367	6.234332947			
Mg	5.406810742	0.870789394	6.234573739			
O	6.909487868	1.721158834	7.291019674			
Mg	0.891266602	3.456098694	6.232804196			
O	-0.596731515	4.334676412	7.283678167			
Mg	-2.104423753	3.462127079	6.265607610			
O	0.889526356	6.937163186	7.256756571			
Mg	-0.610220581	6.062436844	6.229192599			
O	-2.103509687	6.939150801	7.282787618			
Mg	-3.599022514	6.060941531	6.229830120			
O	2.402623000	2.600975000	4.879260000	0	0	0
Mg	0.900878000	1.733758000	3.841750000	0	0	0
O	-0.600924000	2.600863000	4.879265000	0	0	0
Mg	-0.600791000	4.334803000	3.841724000	0	0	0
O	-2.102595000	5.201843000	4.879235000	0	0	0
Mg	-2.102631000	6.936104000	3.841859000	0	0	0
Mg	3.904276000	1.733799000	3.841785000	0	0	0
O	5.406035000	2.601007000	4.879159000	0	0	0
Mg	6.907937000	1.733940000	3.841856000	0	0	0
O	6.907882000	-0.000250000	4.879037000	0	0	0
Mg	2.402608000	4.334844000	3.841761000	0	0	0
O	3.904364000	5.201988000	4.879131000	0	0	0
Mg	3.904427000	6.936284000	3.841965000	0	0	0
O	3.904470000	-0.000282000	4.879136000	0	0	0
O	0.900954000	5.201956000	4.879230000	0	0	0
Mg	0.900768000	6.936143000	3.841896000	0	0	0
O	0.900922000	-0.000394000	4.879140000	0	0	0
Mg	5.406267000	4.334985000	3.841828000	0	0	0
O	0.900998000	3.467942000	2.480698000	0	0	0
Mg	-0.600804000	2.600880000	1.401124000	0	0	0
O	-2.102631000	3.467797000	2.480596000	0	0	0
Mg	-2.102476000	5.201910000	1.401120000	0	0	0
O	-3.604312000	6.068961000	2.480542000	0	0	0
Mg	2.402597000	2.600928000	1.401025000	0	0	0
O	3.904352000	3.467957000	2.480721000	0	0	0
Mg	5.406136000	2.601028000	1.401090000	0	0	0
O	5.406038000	0.866913000	2.480654000	0	0	0
Mg	6.907841000	-0.000119000	1.401206000	0	0	0
Mg	0.900926000	5.201959000	1.401021000	0	0	0
O	2.402671000	6.069120000	2.480668000	0	0	0
Mg	3.904465000	5.202059000	1.401086000	0	0	0
O	2.402683000	0.866897000	2.480632000	0	0	0
Mg	0.900902000	-0.000266000	1.401241000	0	0	0
O	-0.600945000	0.866753000	2.480529000	0	0	0
Mg	3.904302000	-0.000220000	1.401142000	0	0	0
O	-0.600683000	6.069104000	2.480645000	0	0	0
H	2.389157039	2.748594010	12.907332318			
H	2.414782589	6.070832393	13.670879974			
H	5.277739192	7.651581319	12.898553731			
H	-0.466967786	7.695756940	12.903329741			

Structure – (111)/O—CH_4^{Str2}

CELL_PARAMETERS {alat=9.013}

1.000000000000d0	0.000000000000d0	0.000000000000d0
-0.500001664841d0	0.866026923807d0	0.000000000000d0
0.000000000000d0	0.000000000000d0	2.885724333438d0

Starting geometry of (111)/O—CH_4^{Str2}

O	2.402623	2.600927	11.948442
Mg	3.904355	1.733861	11.067329
O	3.904553	-0.000181	11.948245
Mg	2.402661	4.334890	11.067307
O	0.900976	5.201881	11.948392
Mg	0.900733	6.936092	11.067464
Mg	0.900833	1.733811	11.067295
O	0.900970	-0.000361	11.948064
O	3.904302	5.201909	11.948299
Mg	5.406317	4.335066	11.067464
O	5.405960	2.600948	11.948345
Mg	6.908054	1.734057	11.067516
O	6.907882	-0.000157	11.948146
Mg	3.904318	6.936320	11.067619
O	-0.600949	2.600743	11.948254
Mg	-0.600749	4.334741	11.067273
O	-2.102599	5.201698	11.948220
Mg	-2.102763	6.936039	11.067397
O	-0.600683	6.069137	9.659879
Mg	-2.102495	5.201909	8.639976
O	-2.102622	3.467762	9.659832
Mg	-0.600823	2.600874	8.640045
O	-0.600952	0.866728	9.659776
Mg	0.900870	-0.000457	8.640083
O	2.402668	0.866848	9.659798
Mg	3.904350	-0.000395	8.639980
O	5.406046	0.866878	9.659819
Mg	6.907939	-0.000258	8.639992
Mg	0.900977	5.201977	8.639892
O	0.900989	3.467889	9.659861
Mg	2.402631	2.600953	8.639933
O	3.904367	3.467922	9.659877
Mg	5.406229	2.601087	8.639928
O	2.402688	6.069170	9.659902
Mg	3.904547	5.202125	8.639882
O	-3.604308	6.069014	9.659851
O	5.406271	4.334824	7.275808
Mg	3.904402	3.467956	6.240769
O	3.904269	1.733841	7.275939
Mg	5.406084	0.866672	6.240741
O	6.907942	1.733834	7.275841
O	2.402598	4.334831	7.275908
Mg	0.901004	3.467912	6.240733
O	0.900916	1.733827	7.275934
Mg	-0.600996	0.866632	6.240831
Mg	2.402722	6.069084	6.240884
O	0.900884	6.936143	7.275853
Mg	-0.600675	6.069041	6.240842
O	-2.102469	6.936128	7.275846
Mg	-3.604356	6.069042	6.240970

O	3.904556	6.936137	7.275754	
O	-0.600754	4.334816	7.275902	
Mg	-2.102672	3.467911	6.240857	
Mg	2.402681	0.866632	6.240702	
O	2.402624	2.600974	4.879260	0 0 0
Mg	3.904278	1.733798	3.841785	0 0 0
O	3.904472	-0.000283	4.879136	0 0 0
Mg	2.402609	4.334843	3.841761	0 0 0
O	0.900955	5.201954	4.879230	0 0 0
Mg	0.900769	6.936141	3.841896	0 0 0
Mg	0.900880	1.733757	3.841750	0 0 0
O	0.900924	-0.000396	4.879140	0 0 0
O	3.904365	5.201987	4.879131	0 0 0
Mg	5.406268	4.334984	3.841829	0 0 0
O	5.406036	2.601006	4.879160	0 0 0
Mg	6.907938	1.733939	3.841857	0 0 0
O	6.907883	-0.000251	4.879038	0 0 0
Mg	3.904428	6.936283	3.841965	0 0 0
O	-0.600923	2.600861	4.879264	0 0 0
Mg	-0.600790	4.334802	3.841723	0 0 0
O	-2.102594	5.201841	4.879234	0 0 0
Mg	-2.102630	6.936102	3.841858	0 0 0
O	0.901000	3.467940	2.480698	0 0 0
Mg	2.402599	2.600926	1.401025	0 0 0
O	2.402685	0.866895	2.480632	0 0 0
Mg	3.904304	-0.000222	1.401143	0 0 0
O	5.406039	0.866911	2.480655	0 0 0
Mg	6.907843	-0.000121	1.401207	0 0 0
Mg	0.900928	5.201957	1.401020	0 0 0
O	-0.600681	6.069102	2.480644	0 0 0
Mg	-2.102474	5.201908	1.401119	0 0 0
O	-3.604310	6.068959	2.480540	0 0 0
Mg	-0.600802	2.600878	1.401123	0 0 0
O	-0.600943	0.866751	2.480529	0 0 0
Mg	0.900904	-0.000268	1.401241	0 0 0
O	2.402673	6.069118	2.480667	0 0 0
Mg	3.904467	5.202057	1.401086	0 0 0
O	3.904354	3.467955	2.480721	0 0 0
Mg	5.406138	2.601026	1.401090	0 0 0
O	-2.102629	3.467795	2.480595	0 0 0
C	2.402623	2.600927	14.098442	
H	3.240061	3.084454	14.599262	
H	1.714566	2.203651	14.843204	
H	1.883328	3.327828	13.475651	
H	2.772537	1.787775	13.475651	

Final geometry of (111)/O—CH_4^{Str2}

O	2.423224075	2.597762138	11.945171795
Mg	3.997230734	1.697139056	11.079909756
O	3.686705239	0.052792968	12.113674843
Mg	2.374765307	4.412663045	11.077330348
O	0.771075452	4.855107226	12.167784275
Mg	0.659841480	6.727229310	12.386616366
Mg	1.032210608	1.759094741	10.841716891
O	0.433333767	0.444578401	12.263016664
O	3.885031656	5.244459285	11.990889139
Mg	5.424681660	4.335762804	11.218201835
O	5.505692670	2.553608023	12.005310000
Mg	6.842406436	1.591520756	11.013501873

O	6.726536593	-0.133050945	11.923671300			
Mg	3.815130959	6.937674972	11.063743240			
O	-0.346219552	1.718706880	12.334648217			
Mg	-0.615083634	4.426200362	10.913488119			
O	-2.016144025	5.259306202	11.999308789			
Mg	-2.034679900	6.914406352	10.953699851			
O	-0.650783371	6.037904852	9.613470787			
Mg	-2.120432016	5.201079671	8.614437865			
O	-2.036469533	3.457078750	9.728481867			
Mg	-0.607585188	2.594106952	8.594041348			
O	-0.595675520	0.887357400	9.701763391			
Mg	0.889460376	-0.006897150	8.595841963			
O	2.389179043	0.858505559	9.665422273			
Mg	3.953273007	-0.007233066	8.681795056			
O	5.408651956	0.954899315	9.619501166			
Mg	6.876021315	-0.034470871	8.692474061			
Mg	0.918660526	5.234534785	8.670099751			
O	0.890839280	3.438659705	9.682330356			
Mg	2.453989790	2.623889273	8.601896027			
O	3.921017668	3.465699589	9.695777580			
Mg	5.430660141	2.642004904	8.654786471			
O	2.471229617	6.011653453	9.637028703			
Mg	3.951364302	5.193293174	8.672898404			
O	-3.583177508	6.134046520	9.736349081			
O	5.422200477	4.344595499	7.302343635			
Mg	3.913430545	3.471853057	6.235928216			
O	3.898912515	1.745772092	7.270462530			
Mg	5.412388334	0.872553790	6.260052404			
O	6.922908620	1.751577798	7.271463812			
O	2.410253938	4.322328513	7.275732488			
Mg	0.905274182	3.469776202	6.236918750			
O	0.900125737	1.730825011	7.277547322			
Mg	-0.607152687	0.863613565	6.235307856			
Mg	2.411961392	6.068301832	6.259040050			
O	0.910608439	6.938558172	7.289090621			
Mg	-0.595207889	6.072339918	6.251712409			
O	-2.113222251	6.936608103	7.269161503			
Mg	-3.602255800	6.073968298	6.226194871			
O	3.922626781	6.940081484	7.282664765			
O	-0.599718949	4.325655243	7.270288567			
Mg	-2.095576227	3.471372188	6.223653637			
Mg	2.409249891	0.864587696	6.239447299			
O	2.402624000	2.600974000	4.879260000	0	0	0
Mg	3.904278000	1.733798000	3.841785000	0	0	0
O	3.904472000	-0.000283000	4.879136000	0	0	0
Mg	2.402609000	4.334843000	3.841761000	0	0	0
O	0.900955000	5.201954000	4.879230000	0	0	0
Mg	0.900769000	6.936141000	3.841896000	0	0	0
Mg	0.900880000	1.733757000	3.841750000	0	0	0
O	0.900924000	-0.000396000	4.879140000	0	0	0
O	3.904365000	5.201987000	4.879131000	0	0	0
Mg	5.406268000	4.334984000	3.841829000	0	0	0
O	5.406036000	2.601006000	4.879160000	0	0	0
Mg	6.907938000	1.733939000	3.841857000	0	0	0
O	6.907883000	-0.000251000	4.879038000	0	0	0
Mg	3.904428000	6.936283000	3.841965000	0	0	0
O	-0.600923000	2.600861000	4.879264000	0	0	0
Mg	-0.600790000	4.334802000	3.841723000	0	0	0
O	-2.102594000	5.201841000	4.879234000	0	0	0
Mg	-2.102630000	6.936102000	3.841858000	0	0	0

O	0.901000000	3.467940000	2.480698000	0	0	0
Mg	2.402599000	2.600926000	1.401025000	0	0	0
O	2.402685000	0.866895000	2.480632000	0	0	0
Mg	3.904304000	-0.000222000	1.401143000	0	0	0
O	5.406039000	0.866911000	2.480655000	0	0	0
Mg	6.907843000	-0.000121000	1.401207000	0	0	0
Mg	0.900928000	5.201957000	1.401020000	0	0	0
O	-0.600681000	6.069102000	2.480644000	0	0	0
Mg	-2.102474000	5.201908000	1.401119000	0	0	0
O	-3.604310000	6.068959000	2.480540000	0	0	0
Mg	-0.600802000	2.600878000	1.401123000	0	0	0
O	-0.600943000	0.866751000	2.480529000	0	0	0
Mg	0.900904000	-0.000268000	1.401241000	0	0	0
O	2.402673000	6.069118000	2.480667000	0	0	0
Mg	3.904467000	5.202057000	1.401086000	0	0	0
O	3.904354000	3.467955000	2.480721000	0	0	0
Mg	5.406138000	2.601026000	1.401090000	0	0	0
O	-2.102629000	3.467795000	2.480595000	0	0	0
C	2.430768892	2.581231417	13.362847453			
H	3.399112295	2.964104070	13.733693665			
H	-0.049044601	2.100644580	13.190280458			
H	1.633050201	3.258952160	13.734012659			
H	2.287321030	1.544640414	13.720081158			