Stabilization of small organic molecules on V_2C and V_2CO_2 MXenes: First-principles insights into the performance of van der Waals functionals and the effect of oxygen vacancies

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S1. Geometries of adsorbed molecules

CH_4_V_2C

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.111574002	0.222468030	0.102381412
2	V	0.111237791	0.556716262	0.102413830
3	V	0.114624689	0.890991601	0.101824247
4	V	0.448264797	0.222061237	0.102283449
5	V	0.447932403	0.557280034	0.105733711
6	V	0.448523192	0.894385124	0.102344328

7	V	0.781091481	0.224378944	0.102151946
8	V	0.783160205	0.557003104	0.102397828
9	V	0.783096119	0.893848691	0.102433000
10	V	0.226823410	0.116281141	1.000754129
11	V	0.228220259	0.448248901	1.001888752
12	V	0.227053994	0.778006675	1.000758749
13	V	0.559746036	0.113624925	1.000269154
14	V	0.557826768	0.447785211	1.001670128
15	V	0.557348342	0.777310012	1.001894842
16	V	0.891868912	0.113411822	1.000313283
17	V	0.891811517	0.445884556	1.000307993
18	V	0.889075768	0.778343378	1.000819666
19	C	0.003439365	0.001937338	0.050819722
20	C	0.003396348	0.335472044	0.051116435
21	C	0.003406503	0.669102757	0.050687743
22	C	0.336193200	0.001964697	0.050468965
23	C	0.337007008	0.336170959	0.053497658
24	C	0.337054490	0.668449039	0.053866685
25	C	0.669975087	0.002006340	0.051205038
26	C	0.669864374	0.335513855	0.051219722
27	C	0.669187401	0.668383939	0.053628445
28	C	0.440739422	0.555706876	0.229548621
29	H	0.553220289	0.642322969	0.259518290
30	H	0.328179650	0.452964518	0.255899393
31	H	0.488431848	0.486274735	0.197462161
32	H	0.396619092	0.638747331	0.204648782

CH_4_V_2CO_2

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates:

No.	Elements	X	Y	Z
1	V	0.106802512	0.222248874	0.205469280
2	V	0.106646691	0.555372223	0.205500581
3	V	0.106728220	0.888932426	0.205448598
4	V	0.439994684	0.221997460	0.205490905
5	V	0.439792462	0.555313803	0.205361313

6	V	0.440206252	0.888867284	0.205578897
7	V	0.773346816	0.222256805	0.205471161
8	V	0.773647425	0.555689224	0.205415118
9	V	0.773269075	0.888725205	0.205557775
10	V	0.217989639	0.111261285	0.093806143
11	V	0.217832259	0.444447537	0.093782765
12	V	0.217925084	0.777852983	0.093876409
13	V	0.551161491	0.111053970	0.093809666
14	V	0.551345901	0.444494059	0.093855231
15	V	0.551338496	0.777866833	0.093830888
16	V	0.884508964	0.111053993	0.093919519
17	V	0.884572383	0.444587628	0.093799513
18	V	0.884517819	0.777843826	0.093831790
19	C	0.329053920	0.000033712	0.149681361
20	C	0.328911455	0.333230209	0.149618480
21	C	0.328973176	0.666684737	0.149659690
22	C	0.662235114	-0.000062912	0.149703743
23	C	0.662331368	0.333291942	0.149628784
24	C	0.662354868	0.666741220	0.149634222
25	C	0.995631960	-0.000021967	0.149680830
26	C	0.995661320	0.333387527	0.149652425
27	C	0.995677325	0.666680658	0.149642127
28	C	0.439270213	0.440104736	0.387533869
29	O	0.217994676	0.111273957	0.252494323
30	O	0.217792556	0.444433233	0.252413226
31	O	0.217857608	0.777715510	0.252394216
32	O	0.551129000	0.111122596	0.252484739
33	O	0.551515983	0.444455612	0.252034732
34	O	0.551132146	0.777609012	0.252493930
35	O	0.884565672	0.111083376	0.252390481
36	O	0.884490464	0.444532402	0.252451783
37	O	0.884466929	0.777667940	0.252451609
38	O	0.106742964	0.222181035	0.046913390
39	O	0.106767993	0.555545612	0.046887218
40	O	0.106750380	0.888926243	0.046927578
41	O	0.440052031	0.222103054	0.046893461
42	O	0.440028946	0.555588545	0.046933659
43	O	0.440164162	0.888914726	0.046896700
44	O	0.773404440	0.222241797	0.046949433

45	O	0.773532354	0.555653528	0.046876929
46	O	0.773394911	0.888869830	0.046894574
47	H	0.565724800	0.440385492	0.385287984
48	H	0.455071666	0.561180754	0.365499502
49	H	0.400052590	0.436026083	0.436042907
50	H	0.336061305	0.322744928	0.363113696

CH_4_V_2CO_2_Ov

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates:

No.	Elements	X	Y	Z
1	V	0.099324113	0.220291117	0.209475637
2	V	0.094002498	0.547943155	0.210312952
3	V	0.093931757	0.887175642	0.210251918
4	V	0.420088503	0.200045062	0.205815518
5	V	0.419899881	0.561198642	0.205839161
6	V	0.432287344	0.886861812	0.210377801
7	V	0.760652334	0.219854246	0.209505221
8	V	0.781295300	0.561397130	0.205963872
9	V	0.760774622	0.882141627	0.209480086
10	V	0.206540336	0.110520698	0.096864467
11	V	0.206602550	0.437526815	0.096851194
12	V	0.206741348	0.774082898	0.099272039
13	V	0.543998280	0.110256793	0.096860991
14	V	0.540201253	0.440683718	0.100638849
15	V	0.543944348	0.775150555	0.096919746
16	V	0.873873212	0.107605367	0.100571254
17	V	0.870746963	0.437439603	0.096904945
18	V	0.870737937	0.774788140	0.096894634
19	C	0.318089327	0.996415481	0.153561326
20	C	0.318723285	0.330078259	0.155060162
21	C	0.318016202	0.662992868	0.153583607

22	C	0.649843368	0.995651608	0.154178167
23	C	0.651192633	0.330035048	0.155081775
24	C	0.651154026	0.662422375	0.155067988
25	C	0.985531620	0.995691581	0.154156742
26	C	0.985539362	0.331236205	0.154175288
27	C	0.984743612	0.662966690	0.153599916
28	C	0.534978628	0.434867043	0.360914593
29	O	0.211157117	0.110519299	0.257695510
30	O	0.211348006	0.441951708	0.257758924
31	O	0.206870366	0.774103820	0.256116290
32	O	0.539119847	0.110728284	0.257768555
33	O	0.539255506	0.770077009	0.257727767
34	O	0.873844138	0.107605249	0.255436138
35	O	0.870257289	0.441812570	0.257730890
36	O	0.870310826	0.769813439	0.257735745
37	O	0.095552386	0.218530407	0.050145710
38	O	0.095339136	0.550909439	0.051509037
39	O	0.095386624	0.885817720	0.051508588
40	O	0.429531006	0.219124731	0.051431837
41	O	0.429583287	0.551752205	0.051474978
42	O	0.430006803	0.885652518	0.051498960
43	O	0.762767772	0.218444044	0.050162962
44	O	0.762092431	0.551687240	0.051460348
45	O	0.762721782	0.885616587	0.050160392
46	H	0.643411100	0.406970811	0.352410718
47	H	0.563313634	0.559278193	0.337845263
48	H	0.524430040	0.451245232	0.410851517
49	H	0.408179358	0.323672387	0.344452575

CO_2_V_2C

Simulation cell vectors (Å):

a =	8.612000465	0.000000000	0.000000000
b =	-4.306000233	7.458211180	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates:

No.	Elements	X	Y	Z
1	V	0.116172441	0.229760426	0.103844819
2	V	0.115129777	0.564159641	0.105810043
3	V	0.113421122	0.897513290	0.104573613
4	V	0.450599441	0.235941248	0.105352445
5	V	0.453494538	0.556111502	0.107688123
6	V	0.442591855	0.894915414	0.105198843
7	V	0.767943590	0.238528398	0.105974342
8	V	0.771820792	0.558061276	0.106321614
9	V	0.775685052	0.889130936	0.103624797
10	V	0.221722282	0.113890016	0.003551355
11	V	0.220399545	0.451989078	0.004242534
12	V	0.222946369	0.780861070	0.003620989
13	V	0.553895528	0.109926484	0.002772596
14	V	0.553147180	0.453078366	1.000356570
15	V	0.553054479	0.785538556	0.004295804
16	V	0.888540006	0.119291727	0.005312838
17	V	0.899221596	0.454746663	0.003461210
18	V	0.894477032	0.785064259	0.003746640
19	C	-0.000212728	0.006524926	0.054053045
20	C	-0.001497072	0.339276998	0.056836001
21	C	0.001666259	0.673103749	0.055718840
22	C	0.333422943	0.004480300	0.053756147
23	C	0.335382765	0.340430858	0.051135158
24	C	0.336293746	0.671475012	0.056652386
25	C	0.667232953	0.007625984	0.056262202
26	C	0.666160421	0.342120304	0.045465666
27	C	0.666631014	0.672231499	0.050164552
28	C	0.556354442	0.421294434	0.170951291
29	O	0.684896476	0.355037189	0.171382126
30	O	0.628235380	0.588670527	0.187839663

CO_2_V_2CO_2

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.109655946	0.227967191	0.205447939
2	V	0.109722820	0.561104723	0.205790930
3	V	0.109953081	0.895209408	0.205627636
4	V	0.442925314	0.228097858	0.205733896
5	V	0.443104988	0.561960764	0.205210610
6	V	0.443161370	0.894969380	0.205704436
7	V	0.776342954	0.228249071	0.205555676
8	V	0.776646879	0.561452205	0.205652880
9	V	0.776256899	0.894528342	0.205672293
10	V	0.220949675	0.117179156	0.093905806
11	V	0.220659629	0.450229808	0.093808946
12	V	0.220763080	0.783446503	0.094231823
13	V	0.553966073	0.117056603	0.093916498
14	V	0.554501753	0.450556657	0.094003008
15	V	0.554241214	0.783950839	0.093818829
16	V	0.887517345	0.117143587	0.093939618
17	V	0.887738123	0.450457545	0.093988914
18	V	0.887474307	0.783588956	0.093911705
19	C	0.332089390	0.006178481	0.149790191
20	C	0.331896575	0.339307728	0.149740479
21	C	0.331883891	0.672395104	0.149708445
22	C	0.665356114	0.005934492	0.149772299
23	C	0.665350192	0.339327806	0.149814369
24	C	0.665541777	0.672808106	0.149716852
25	C	0.998420441	0.005860812	0.149723633
26	C	0.998716680	0.339295020	0.149755351
27	C	0.998455071	0.672376989	0.149833795
28	C	0.428767075	0.455698017	0.379327110
29	O	0.220858480	0.117320083	0.252563025
30	O	0.220980119	0.449734621	0.252629437
31	O	0.220707297	0.783495904	0.252460499
32	O	0.554414971	0.117314002	0.252470727
33	O	0.554440451	0.450969130	0.252571680
34	O	0.554721344	0.784159744	0.252266639
35	O	0.887531364	0.116953621	0.252390333
36	O	0.887287315	0.450288913	0.252556074

37	O	0.887339890	0.783499665	0.252562303
38	O	0.109893804	0.228141240	0.046953651
39	O	0.109846139	0.561637449	0.046993007
40	O	0.109868979	0.894955797	0.047112245
41	O	0.443018938	0.228112115	0.046986542
42	O	0.442924462	0.561496418	0.046954209
43	O	0.442806960	0.894725208	0.046997447
44	O	0.776383621	0.228103617	0.047066872
45	O	0.776550371	0.561397263	0.046959509
46	O	0.776510724	0.894751022	0.046947296
47	O	0.416402183	0.314991658	0.382546780
48	O	0.440919615	0.596460419	0.376443132

CO_2_V_2CO_2_Ov

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.107575830	0.221219083	0.209677090
2	V	0.100918780	0.545955267	0.211915762
3	V	0.100606898	0.889384256	0.212023898
4	V	0.424914922	0.193693427	0.207082795
5	V	0.425082597	0.565384313	0.206833874
6	V	0.445113321	0.889598349	0.212050049
7	V	0.769878610	0.221238738	0.209638555
8	V	0.796157750	0.565311605	0.206595638
9	V	0.770058877	0.883719530	0.209526252
10	V	0.215257835	0.110810640	0.097201203
11	V	0.215508583	0.439458523	0.097189335
12	V	0.215760026	0.775207817	0.101354949
13	V	0.551712850	0.110893197	0.097141783
14	V	0.548720424	0.441433118	0.103247714

15	V	0.551558654	0.775461777	0.097126028
16	V	0.882394679	0.108622628	0.101700066
17	V	0.880222103	0.439568083	0.097157023
18	V	0.880152943	0.775470719	0.097073640
19	C	0.325840026	0.995454001	0.154323208
20	C	0.328326630	0.331399293	0.157158346
21	C	0.325847335	0.665100254	0.154238026
22	C	0.658504300	0.996638939	0.155049425
23	C	0.659163684	0.331255816	0.157083609
24	C	0.659398896	0.662708892	0.156978518
25	C	0.994294647	0.996610054	0.155049557
26	C	0.994282236	0.332395170	0.155061987
27	C	0.995497764	0.665157175	0.154156209
28	C	0.575943242	0.474740185	0.336813169
29	O	0.218061726	0.109198591	0.259548297
30	O	0.218168310	0.443726076	0.259573911
31	O	0.215725230	0.775222002	0.256111656
32	O	0.547384300	0.109329143	0.259598055
33	O	0.547416110	0.772386485	0.259678348
34	O	0.882215110	0.108395669	0.256327299
35	O	0.881403600	0.443825764	0.259610488
36	O	0.881102970	0.772156802	0.259712061
37	O	0.10464086	0.219759517	0.051544204
38	O	0.10414268	0.552073947	0.052185415
39	O	0.10424917	0.886837838	0.052202874
40	O	0.43851678	0.220977133	0.052463271
41	O	0.43868066	0.552174101	0.052481584
42	O	0.43884658	0.886787048	0.052212428
43	O	0.77127670	0.219715281	0.051533042
44	O	0.76955913	0.552107402	0.052463929
45	O	0.77131524	0.886394437	0.051518069
46	O	0.55198365	0.446137476	0.282647733
47	O	0.59839240	0.501375535	0.389353746

H_2_V_2C

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000

b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.116210923	0.220855884	0.104302963
2	V	0.113955495	0.554510171	0.104126356
3	V	0.114517036	0.886400665	0.103837528
4	V	0.445542524	0.219314731	0.103622648
5	V	0.447629364	0.552853057	0.104135842
6	V	0.445699965	0.887015806	0.103802206
7	V	0.779514394	0.219861634	0.104300496
8	V	0.779187872	0.554517226	0.103884323
9	V	0.778458637	0.883244632	0.104226749
10	V	0.222818864	0.107531210	0.002080764
11	V	0.222362776	0.441699801	0.002332686
12	V	0.224127227	0.774694403	0.002116389
13	V	0.559180801	0.109150306	0.002324928
14	V	0.558581631	0.440749498	0.001950224
15	V	0.557765040	0.777315172	0.002222049
16	V	0.891501710	0.108996168	0.003038986
17	V	0.89134065	0.441307860	0.002686142
18	V	0.89325525	0.776981011	0.002127332
19	C	0.00205513	-0.002534019	0.054058103
20	C	0.00244838	0.330864054	0.054338413
21	C	0.00186226	0.664157765	0.053223354
22	C	0.33567674	-0.002197397	0.052496422
23	C	0.33565220	0.330760459	0.051962680
24	C	0.33583046	0.664244682	0.053050236
25	C	0.66919563	-0.002524670	0.054011882
26	C	0.66900801	0.331160886	0.053746711
27	C	0.66943317	0.664504812	0.051501936
28	H	0.38349170	0.510167706	0.183644893
29	H	0.49692075	0.597604229	0.184605501

H_2_V_2CO_2

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.1065497303	0.2232736564	0.2058053799
2	V	0.1065660588	0.5565389400	0.2058187309
3	V	0.1065863467	0.8899316987	0.2058369115
4	V	0.4399222265	0.2232873362	0.2058086479
5	V	0.4398537096	0.5565664618	0.2058524608
6	V	0.4397798287	0.8899495842	0.2057635112
7	V	0.7732349161	0.2232262156	0.2058273763
8	V	0.7733089032	0.5566010510	0.2058249402
9	V	0.7732642595	0.8899390623	0.2057727014
10	V	0.2176990551	0.1121142180	0.0941432207
11	V	0.2177314160	0.4454602827	0.0941875101
12	V	0.2176082391	0.7787703202	0.0941449539
13	V	0.5509939207	0.1121101260	0.0941398044
14	V	0.5510490483	0.4455633941	0.0941641234
15	V	0.5510221938	0.7787825714	0.0941838944
16	V	0.8843303836	0.1120734140	0.0941698775
17	V	0.8842779707	0.4454024701	0.0941915466
18	V	0.8842915133	0.7787936249	0.0941837673
19	C	0.3287420600	0.0010318592	0.1499609757
20	C	0.3288014123	0.3343535206	0.1499834560
21	C	0.3287790036	0.6676912309	0.1499841108
22	C	0.6621025983	0.0010389985	0.1499659971
23	C	0.6621067007	0.3343343577	0.1499959341
24	C	0.6620963163	0.6676779586	0.1499977280
25	C	0.9955021369	0.0010388028	0.1499819794
26	C	0.9954331424	0.3343403363	0.1500080394
27	C	0.9954686431	0.6676938123	0.1500091868
28	O	0.2177275331	0.1121791589	0.2527567102
29	O	0.2176156910	0.4454132355	0.2527518227
30	O	0.2176933237	0.7787952638	0.2527759121
31	O	0.5509953931	0.1121133913	0.2527673728
32	O	0.5510339188	0.4453200765	0.2527042717

33	O	0.5510841182	0.7790751607	0.2526821204
34	O	0.8843087282	0.1121054112	0.2527594092
35	O	0.8843171551	0.4454421028	0.2527441398
36	O	0.8843142519	0.7788266757	0.2527692480
37	O	0.1065713342	0.2232522973	0.0472416260
38	O	0.1065410790	0.5565620073	0.0472561503
39	O	0.1065499201	0.8899161222	0.0472274387
40	O	0.4399026334	0.2232805813	0.0472276771
41	O	0.4398509216	0.5565324341	0.0472390684
42	O	0.4398491185	0.8898985111	0.0472279222
43	O	0.7732202812	0.2232388158	0.0472443487
44	O	0.7732701693	0.5565791396	0.0472472825
45	O	0.7732366387	0.8899124804	0.0472293311
46	H	0.4875357537	0.6301696451	0.3705652443
47	H	0.4567132237	0.5336558022	0.3754686958

H_2_V_2CO_2_Ov

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.106079615	0.222706796	0.209533107
2	V	0.100948455	0.550491873	0.210555955
3	V	0.100921105	0.889749638	0.210525026
4	V	0.426930091	0.202374834	0.205842027
5	V	0.426902087	0.563682591	0.205697076
6	V	0.439801481	0.889493968	0.210556967
7	V	0.767897475	0.222452896	0.209495336
8	V	0.788301370	0.563748814	0.205825069
9	V	0.767692890	0.884400510	0.209584791
10	V	0.213510245	0.112705716	0.096944103
11	V	0.213309579	0.439642428	0.096880150
12	V	0.213877678	0.776449121	0.099354993
13	V	0.550809949	0.112551192	0.096928846
14	V	0.547263504	0.443325015	0.100603497
15	V	0.550980663	0.777347578	0.096897012
16	V	0.880733247	0.109883937	0.100643648
17	V	0.877864232	0.439623885	0.096941125
18	V	0.877867248	0.777088043	0.096899081
19	C	0.324995357	0.998651624	0.153692042
20	C	0.325669142	0.332384788	0.155062222
21	C	0.324986756	0.665481078	0.153656783
22	C	0.656827134	0.997885583	0.154249949
23	C	0.658069183	0.332413279	0.155063953
24	C	0.658234925	0.664883206	0.155062756
25	C	0.992504219	0.997924863	0.154254013
26	C	0.992577685	0.333646487	0.154248163
27	C	0.991944694	0.665558910	0.153681398
28	O	0.218581502	0.113408969	0.257780455
29	O	0.218854914	0.444388645	0.257862422

30	O	0.213926357	0.776516691	0.256249392
31	O	0.546224503	0.113277041	0.257833241
32	O	0.546059573	0.771551467	0.257842090
33	O	0.880696491	0.109870676	0.255484272
34	O	0.876828402	0.444193670	0.257844407
35	O	0.877146482	0.771878300	0.257798135
36	O	0.102479803	0.220737693	0.050198923
37	O	0.102399500	0.553455480	0.051559058
38	O	0.102461734	0.888150090	0.051567364
39	O	0.436440760	0.221454486	0.051489711
40	O	0.436426775	0.554166788	0.051442569
41	O	0.437021381	0.888031965	0.051571724
42	O	0.769678048	0.220763086	0.050226925
43	O	0.769128833	0.554078672	0.051470346
44	O	0.769826708	0.888047114	0.050217480
45	H	0.510444971	0.437499798	0.336311851
46	H	0.579164882	0.408858910	0.336121695

$H_2O\_V_2C$

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.104838435	0.219074794	0.102713642
2	V	0.104146185	0.553475423	0.102933008
3	V	0.108607195	0.889434974	0.102411261
4	V	0.442467203	0.219188546	0.103150423
5	V	0.440792959	0.553733960	0.108144598
6	V	0.442128802	0.892711234	0.103393583
7	V	0.777461470	0.223739261	0.103527792
8	V	0.780379022	0.554818884	0.103361234
9	V	0.781445146	0.893893330	0.103806267
10	V	0.222826962	0.115298926	1.001099702

11	V	0.224417694	0.446751088	0.002811459
12	V	0.222452990	0.775948099	1.001850281
13	V	0.555932213	0.112261540	1.001386954
14	V	0.553131142	0.447281921	0.003295513
15	V	0.553203574	0.774899962	0.003656868
16	V	0.884575466	0.110805679	1.001064663
17	V	0.885106152	0.443036941	1.000848561
18	V	0.881241296	0.774705022	1.001580179
19	C	-0.001352026	-0.000158988	0.050201856
20	C	-0.001770600	0.333540983	0.051158260
21	C	-0.001407664	0.667505182	0.050862255
22	C	0.330809227	-0.000093587	0.050920231
23	C	0.331810442	0.334106668	0.054561736
24	C	0.331983547	0.666205769	0.055225450
25	C	0.664427758	-0.000259586	0.052964170
26	C	0.664465878	0.333419737	0.052500302
27	C	0.663474672	0.666035742	0.056335725
28	O	0.440939799	0.553479557	0.208296259
29	H	0.506385469	0.493678070	0.220797310
30	H	0.316838285	0.477646236	0.220962238

$H_2O\_V_2CO_2$

Simulation cell vectors (Å):

a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

No.	Elements	X	Y	Z
1	V	0.108956607	0.229326436	0.206360903
2	V	0.108342377	0.561874740	0.206229464
3	V	0.108693996	0.896109955	0.206521464
4	V	0.441403303	0.227771032	0.206225946
5	V	0.441639933	0.562733113	0.206185692
6	V	0.442636238	0.896222634	0.206569407
7	V	0.775486965	0.229411267	0.206102789

8	V	0.776095165	0.562900837	0.205934406
9	V	0.775562950	0.895662494	0.206151051
10	V	0.219771549	0.118071200	0.094509263
11	V	0.220076827	0.451419328	0.094505078
12	V	0.220119987	0.784815160	0.094863793
13	V	0.553236213	0.117856704	0.094495425
14	V	0.553240026	0.451434596	0.094899449
15	V	0.553172928	0.784490135	0.094574966
16	V	0.886497705	0.118067873	0.094653617
17	V	0.886377589	0.451418623	0.094488449
18	V	0.886671695	0.784499208	0.094474669
19	C	0.330984152	0.006803645	0.150494399
20	C	0.330844493	0.340163232	0.150509920
21	C	0.331138581	0.673666601	0.150497522
22	C	0.664175635	0.006818025	0.150433484
23	C	0.664262592	0.340065114	0.150432396
24	C	0.664394276	0.673723460	0.150408064
25	C	0.997741992	0.006850699	0.150417654
26	C	0.997745432	0.340296627	0.150387244
27	C	0.997701054	0.673679957	0.150416633
28	O	0.219210480	0.117784663	0.252922166
29	O	0.220000016	0.451324145	0.253265072
30	O	0.219867147	0.784618426	0.253061918
31	O	0.553789370	0.118241469	0.253314322
32	O	0.553893911	0.452026926	0.253390319
33	O	0.553359271	0.784628124	0.253299520
34	O	0.886487379	0.118093690	0.253020660
35	O	0.886158151	0.451280176	0.253287129
36	O	0.886447600	0.784421334	0.253259360
37	O	0.108912843	0.229183064	0.047657496
38	O	0.108760095	0.562366434	0.047781538
39	O	0.108727333	0.895778763	0.047708591
40	O	0.442093749	0.229049069	0.047777111
41	O	0.442040782	0.562470115	0.047676591
42	O	0.442264745	0.895726552	0.047681787
43	O	0.775307059	0.229099687	0.047644787
44	O	0.775453433	0.562507569	0.047632123
45	O	0.775425027	0.895627012	0.047730616
46	O	0.427521545	0.280225192	0.374216591

47	H	0.503285202	0.373898281	0.345393626
48	H	0.507989517	0.261303868	0.400102777

H_2O_V_2CO_2_Ov

Simulation cell vectors (Å):

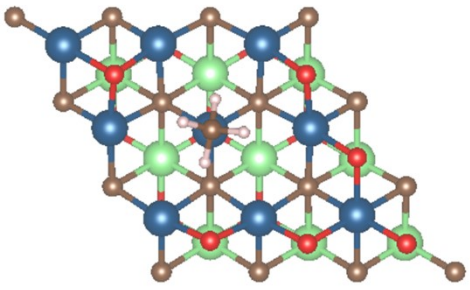
a =	8.612999916	0.000000000	0.000000000
b =	-4.306499958	7.459076730	0.000000000
c =	0.000000000	0.000000000	21.443000794

Fractional coordinates

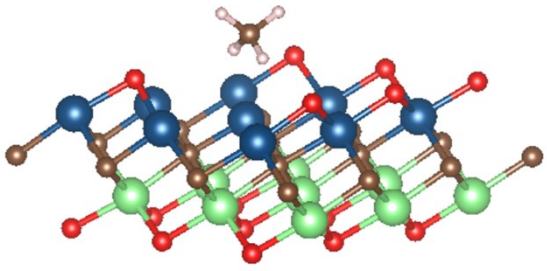
No.	Elements	X	Y	Z
1	V	0.104888734	0.220630471	0.210061314
2	V	0.096083255	0.545380522	0.212270094
3	V	0.096181361	0.887104573	0.212207184
4	V	0.420959182	0.194613635	0.206817347
5	V	0.420762396	0.562733227	0.206431979
6	V	0.441575630	0.889014952	0.213375194
7	V	0.766803930	0.218834546	0.209487364
8	V	0.789177683	0.562748783	0.208590234
9	V	0.766490049	0.883570226	0.209622036
10	V	0.212614615	0.109815536	0.097480504
11	V	0.212272952	0.438450100	0.097184707
12	V	0.211897596	0.774235522	0.101903352
13	V	0.550471165	0.110805041	0.097175982
14	V	0.544725478	0.440477718	0.103372047
15	V	0.550667901	0.776010767	0.097082329
16	V	0.879198706	0.107569033	0.101787100
17	V	0.878121871	0.440932240	0.098402774
18	V	0.878081151	0.773013754	0.098462931
19	C	0.323596490	-0.004881203	0.154843004
20	C	0.324601522	0.330457251	0.156944049
21	C	0.323477891	0.664593743	0.154719177
22	C	0.654927187	-0.004526463	0.155350009
23	C	0.656031700	0.330273670	0.157269480
24	C	0.655973902	0.661838042	0.157237394
25	C	0.991102149	-0.004257339	0.155381316

26	C	0.991245158	0.331561370	0.155312385
27	C	0.992592615	0.664333638	0.155082160
28	O	0.215349032	0.108726227	0.259505978
29	O	0.215817082	0.443034461	0.259446867
30	O	0.212664815	0.774363641	0.256868658
31	O	0.544928307	0.112445011	0.260359048
32	O	0.544543091	0.767817397	0.260282505
33	O	0.878982897	0.107500268	0.256746111
34	O	0.879894339	0.441300661	0.260220259
35	O	0.879760379	0.774452096	0.260218030
36	O	0.101385254	0.218584290	0.051772833
37	O	0.101090690	0.551722033	0.052581684
38	O	0.101070038	0.885683536	0.052594138
39	O	0.435662786	0.219877340	0.052638836
40	O	0.435730367	0.551988544	0.052580241
41	O	0.435371880	0.885791571	0.052880801
42	O	0.769149282	0.220048998	0.051964885
43	O	0.766329411	0.551195718	0.053076045
44	O	0.769322899	0.885150788	0.051948173
45	O	0.575053250	0.452490684	0.284757978
46	H	0.588249044	0.551144383	0.310811993
47	H	0.598516469	0.372463345	0.310156668

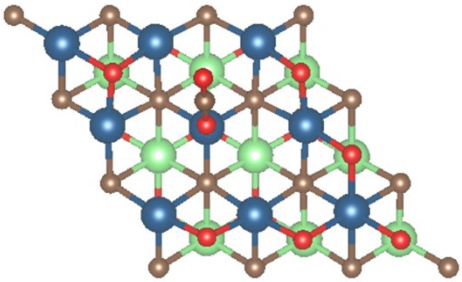
S2. Adsorption configurations at high vacancy regime



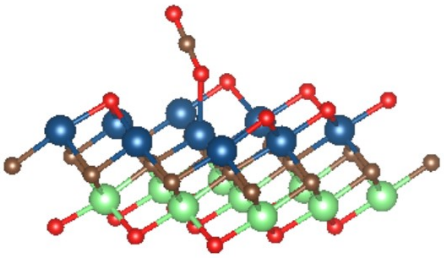
CH_4 top view



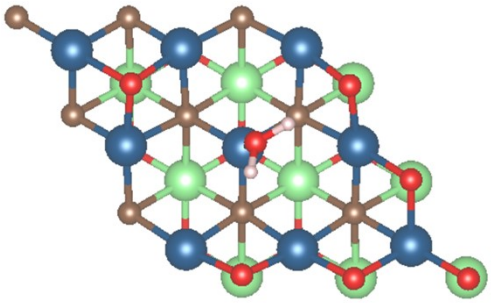
CH_4 side view



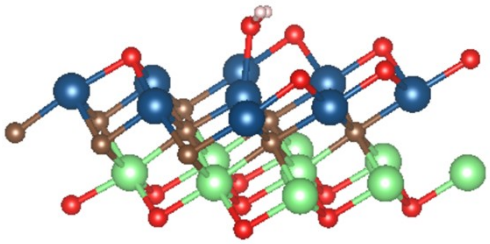
CO_2 top view



CO_2 top view



H_2O top view



H_2O side view