Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The Remarkable Performance of a Single Iridium Atom Supported on Hematite for Methane Activation: A Density Functional Theory Study

Kefale Wagaw Yizengaw [a, b], Tigist Ayalew Abay [a], Delele Worku Ayele [c], Jyh-Chiang Jiang [a],*

[a] Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei city 106, Taiwan

[b] Faculty of Chemical and Food Engineering, Bahir Dar Institute of Technology, Bahir Dar University, Bahir Dar, Ethiopia

[c] Department of Chemistry, College of Science, Bahir Dar University, Bahir Dar, Ethiopia

*Corresponding author. E-mail: jcjiang@mail.ntust.edu.tw (J.-C. Jiang)

Table 1S. Surface energy of the three dominant surface planes of hematite

Surface	Top layer atom type	Surface Energy (eV /Å^2)
110	Fe	0.140
	O	0.108
	O	0.149
	O	0.262
	O	0.232
104	O	0.126
	O	0.129
	Fe	0.259
	Fe	0.143
	O	0.275
012	O	0.112
	O	0.245
	Fe	0.258
	O	0.180
	Fe	0.167

Table 2S. The dopants calculated and experimental lattice parameters, and chemical potential of the

considered dopants in this study.

Substance	Calculated Lattice a=b=c [Å]	Experimental lattice a=b=c [Å]	Chemical potential
Bulk Fe	2.953	2.853[1]	-2.879
Bulk Ir	4.003	3.381[1]	-6.575
Bulk Cu	3.689	3.632[1]	-0.862
Bulk Co	4.194	4.350[2]	-2.003
Bulk Ag	4.076	4.062[1]	-1.809

Table 3S. Adsorption energies of methane for different catalyst surface with and without Van der Waals force consideration.

Surfaces	**Eads (eV)**	
	PBE	**optB88-vdW**
α-Fe_2O_3(110)	-0.041	-0.211
Ir/α-Fe_2O_3(110)	-0.175	-0.395
Ir/α-Fe_2O_3(110)_O_V	-0.328	-0.590

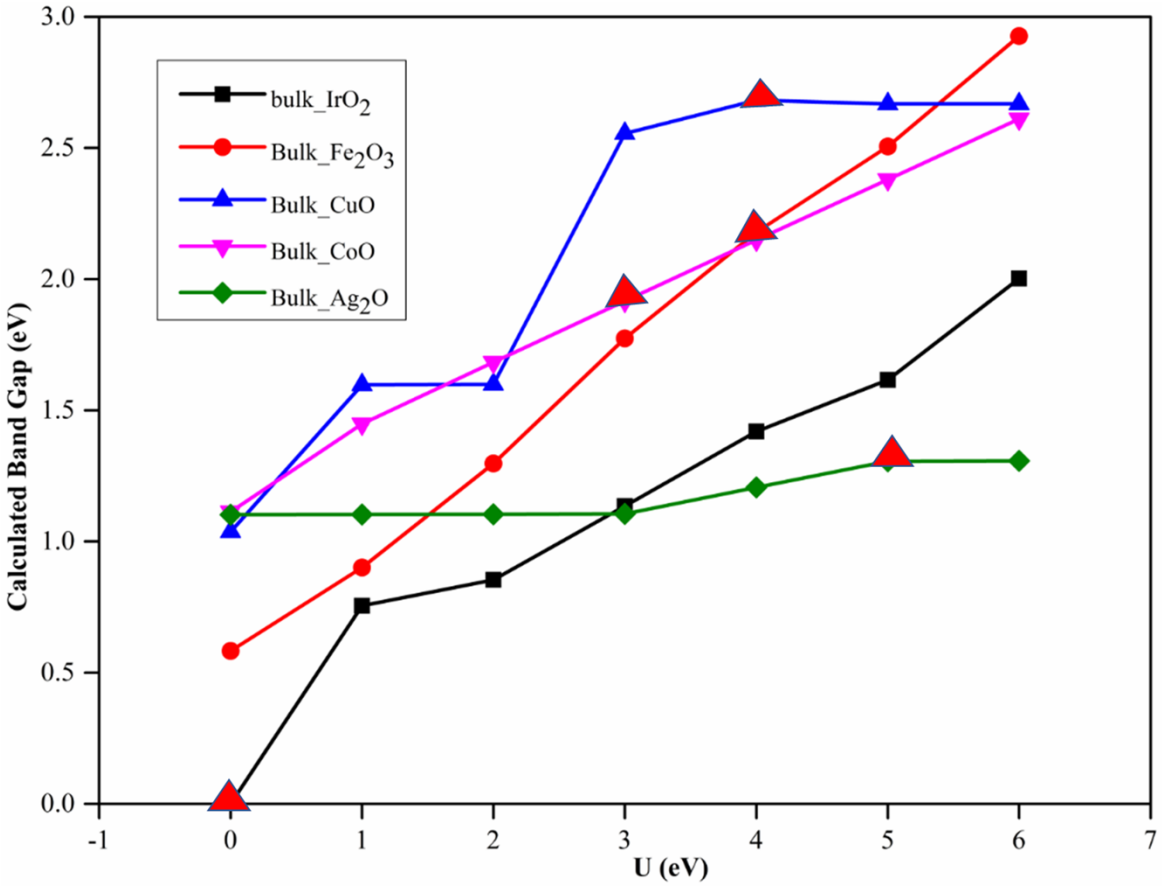

Fig 1S.The calculated DFT +U band gap for the oxides surface as a function of U values. The experimental data are indicated by red color filled triangle.

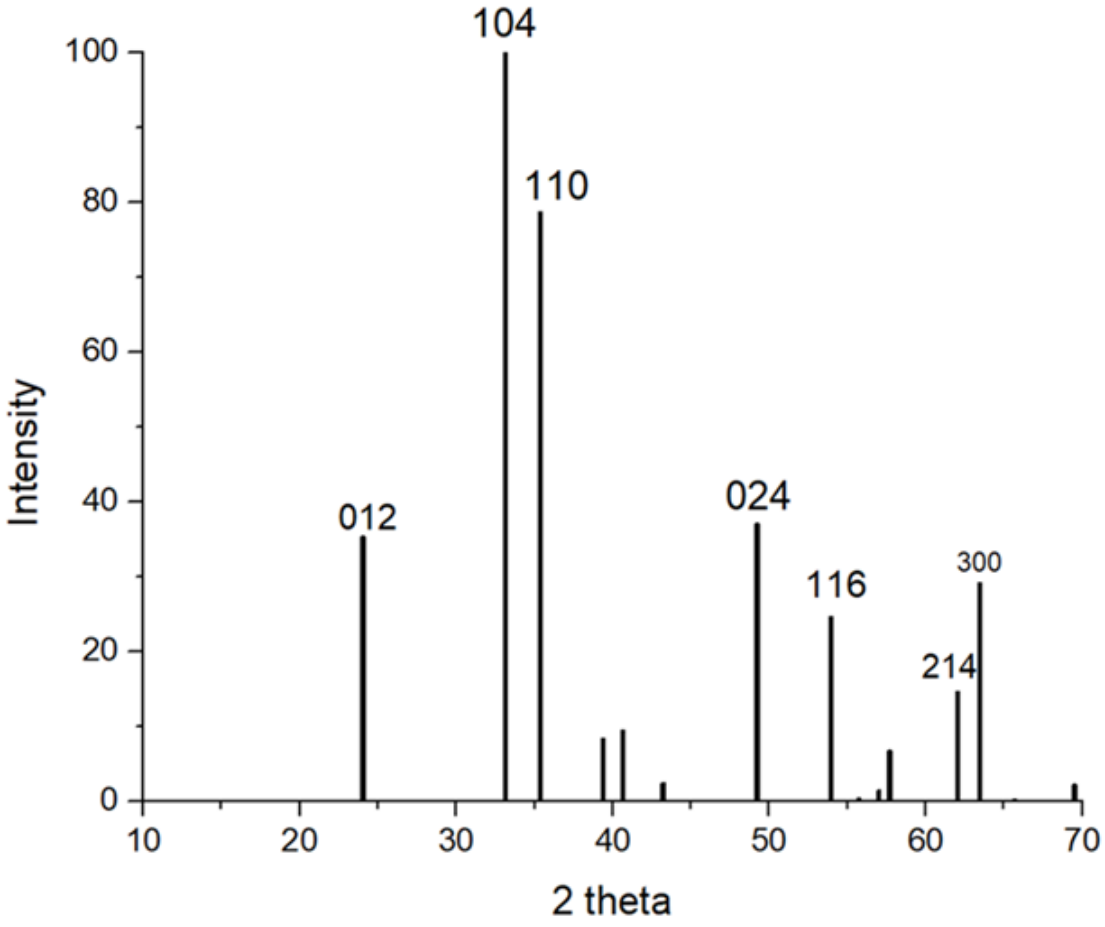

Fig 2S. The calculated x-ray diffraction pattern of hematite (α-Fe_2O_3)

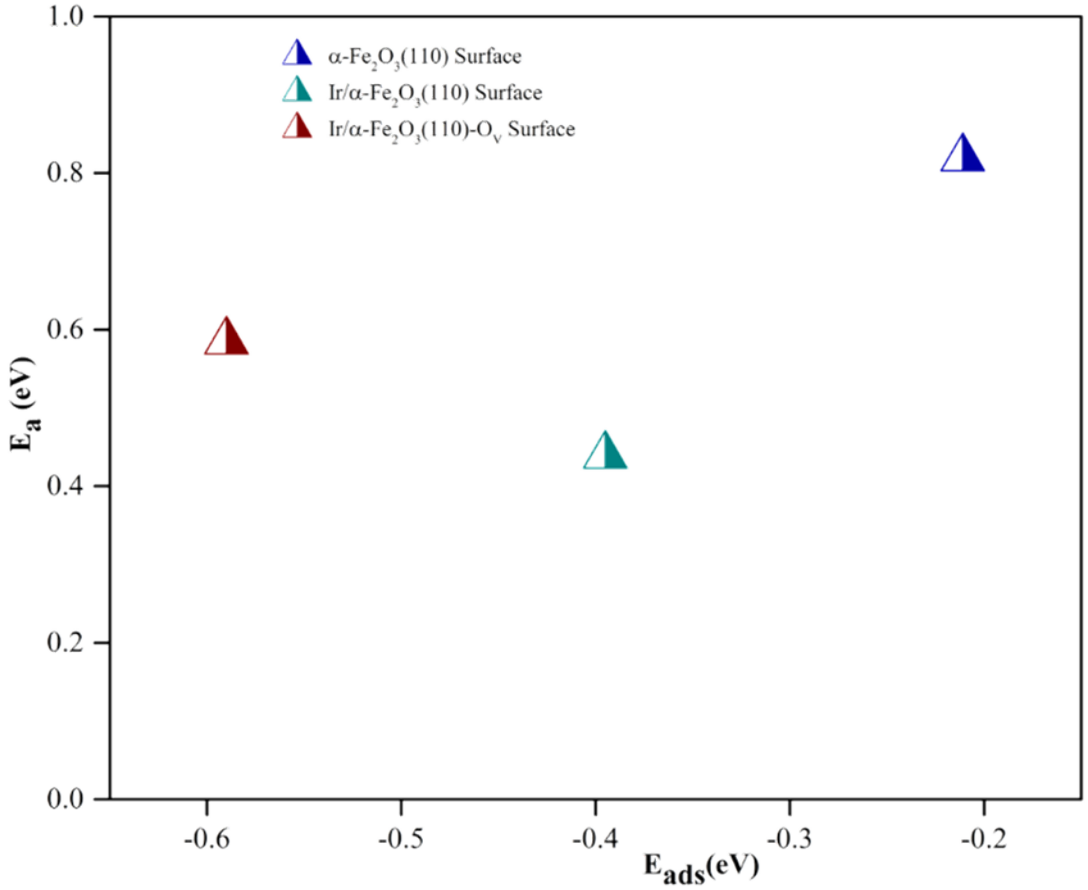

Fig. 3S The plot of the reaction barriers (E_a) against their corresponding adsorption energies (E_{ads}) over α-Fe_2O_3 (110), Ir/α-Fe_2O_3(110), and Ir/α-Fe_2O_3(110)-O_V surfaces

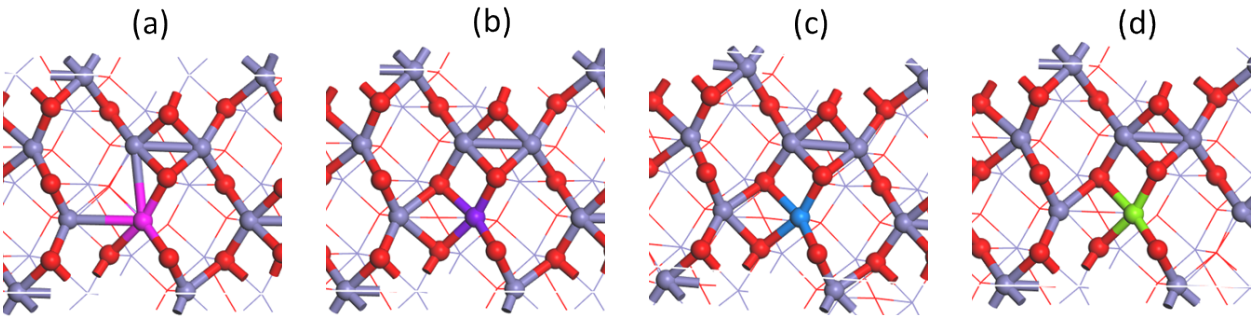

Fig 4S. Single atom dopant on the pristine α-Fe_2O_3(110) surface: (a) Ag/α-Fe_2O_3(110) surface (b) Co/α-Fe_2O_3(110) surface (c) Cu/α-Fe_2O_3(110) surface and (d) Ir/α-Fe_2O_3(110) surface.

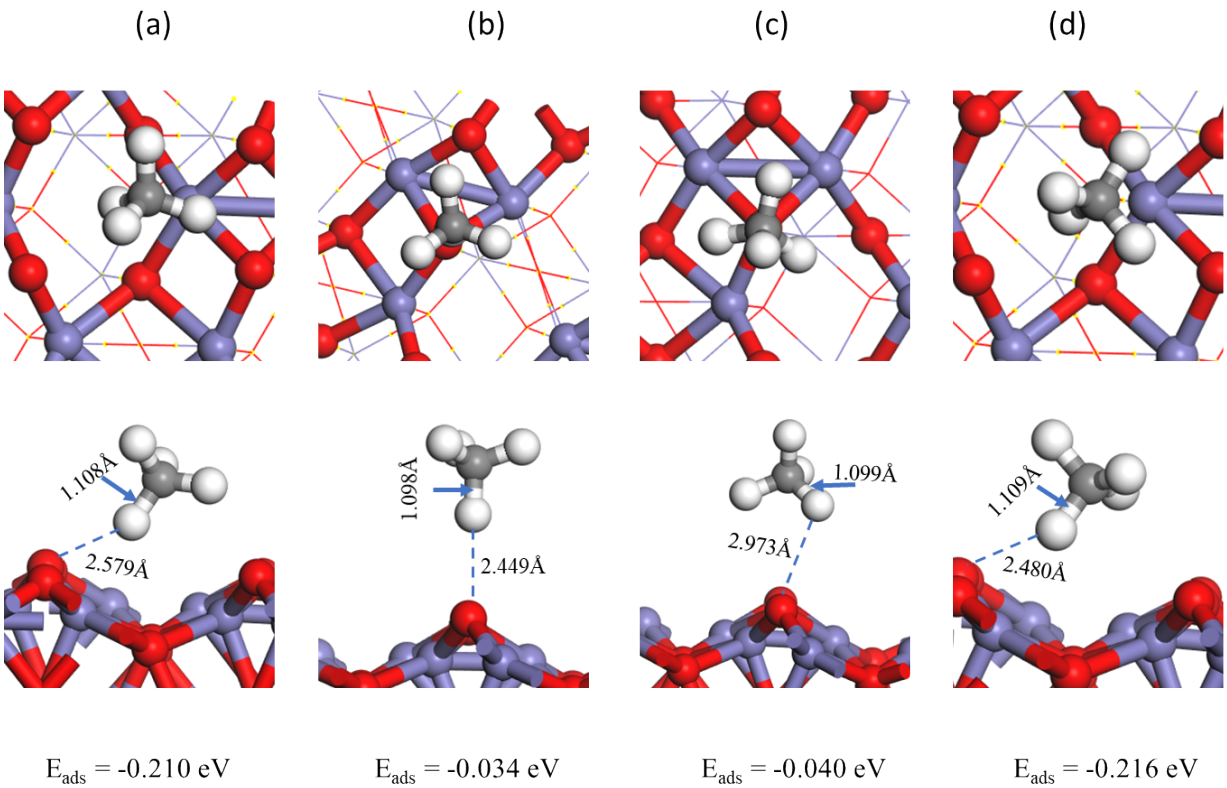

Fig 5S. Optimized geometries for CH_4 adsorption on pristine α-Fe_2O_3(110) surface

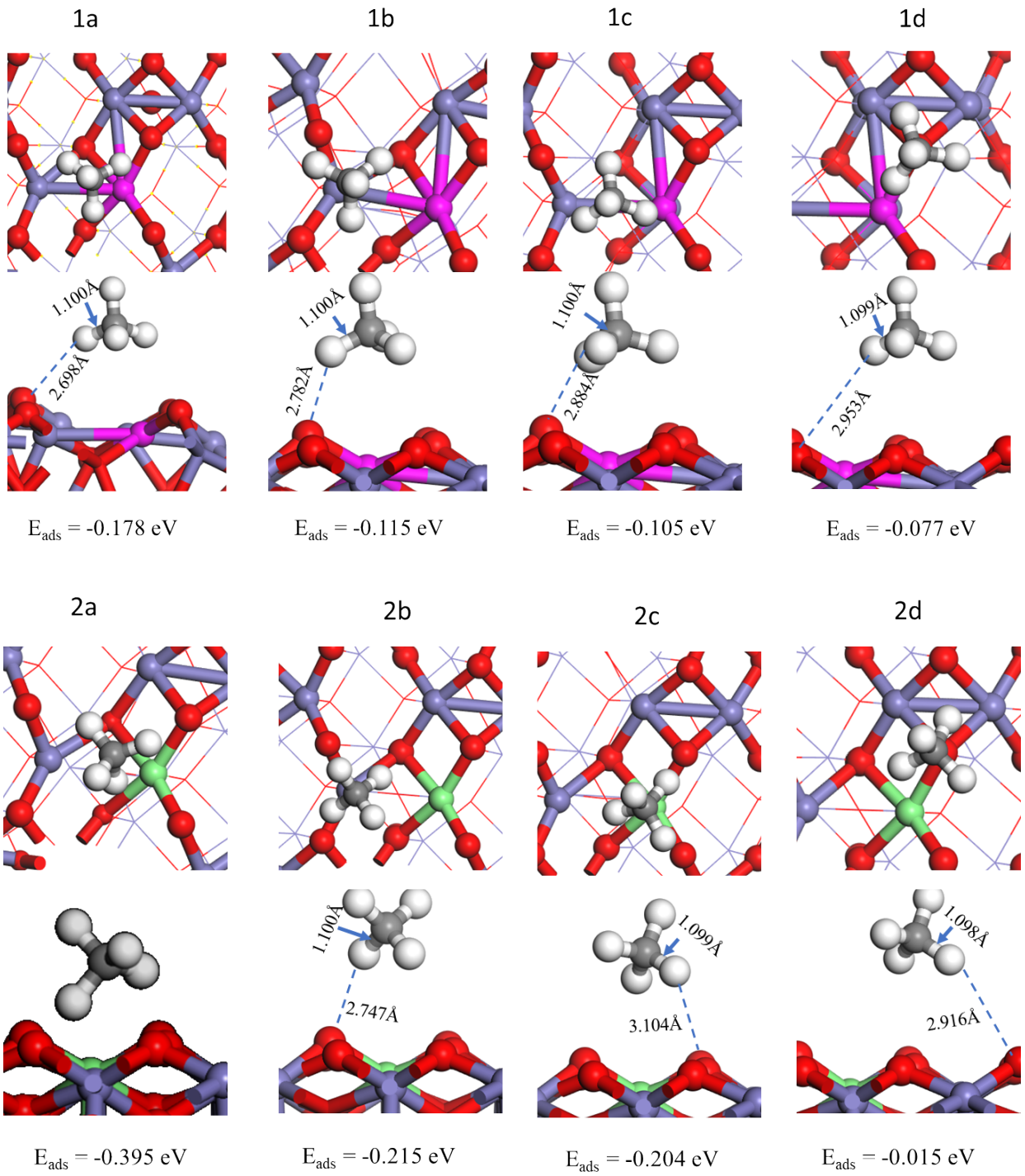

Fig 6S. Optimized geometries for CH_4 adsorption on M/α-Fe_2O_3(110) surfaces

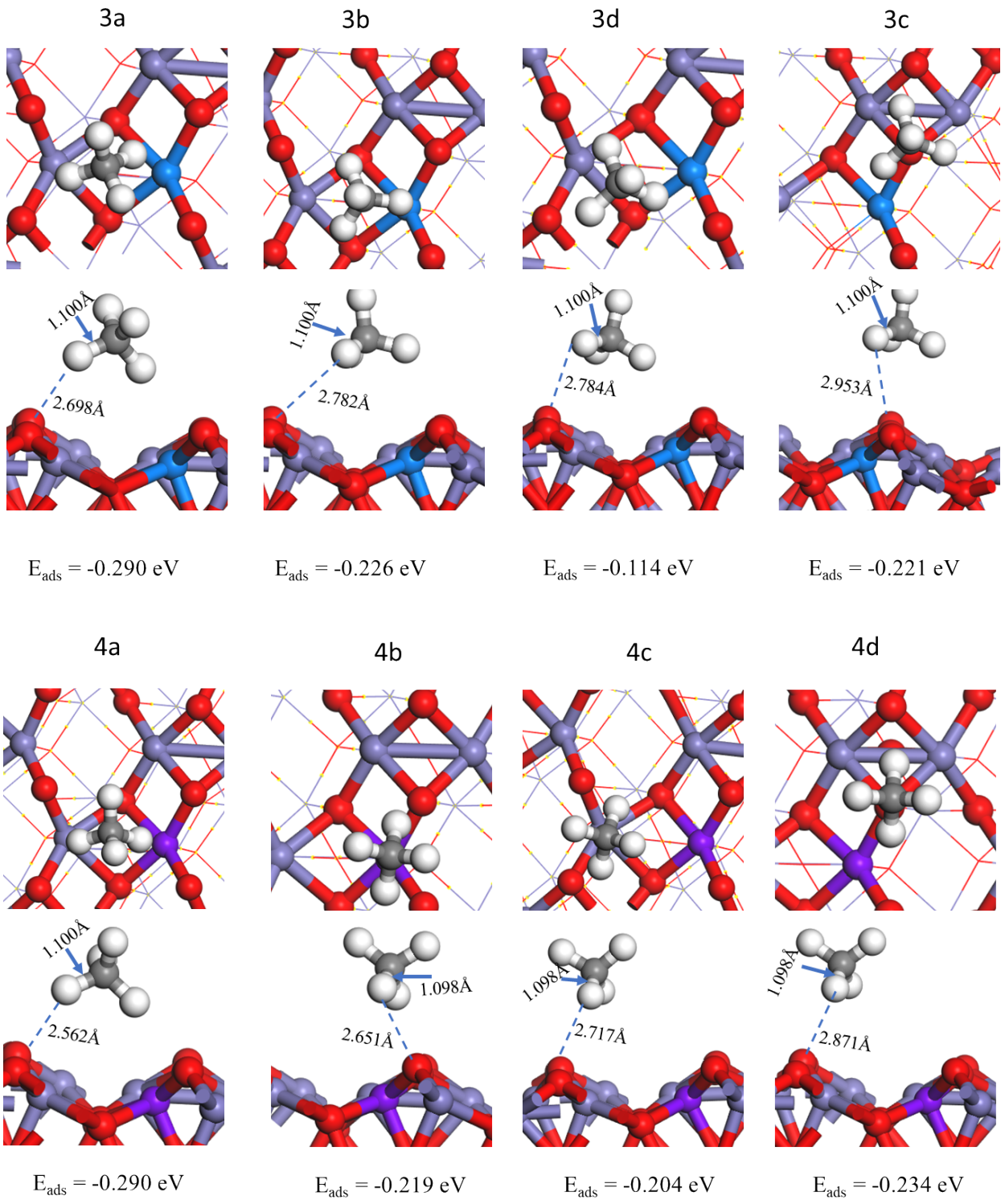

Fig 7S. Optimized geometries for CH_4 adsorption on M/α-Fe_2O_3 (110) surfaces

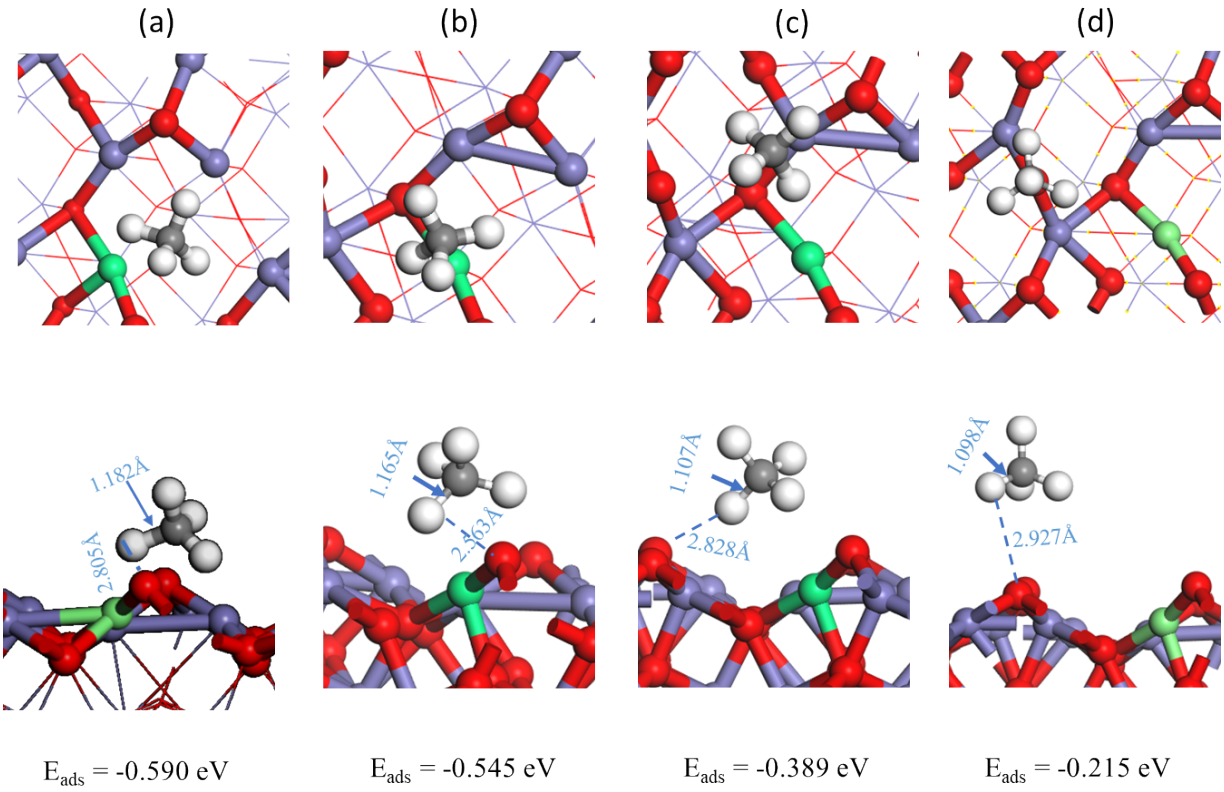

Fig 8S. Optimized geometries for CH_4 adsorption on Ir/α-Fe_2O_3(110)-O_V surfaces

POSCAR coordinates for the structures of the catalyst, reactant, intermediate, product, and transition state were given as follows:

1. Initial structure of methane adsorption on α-Fe_2O_3(110) surface:

a =13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605°

C	Fe	H	O
1	36	4	54

0.4226525265063452	0.6856781031428607	0.4530193309706322
0.9791200160000031	0.6666700239999983	0.0444899980000031
0.9802725395123421	0.1644339017724123	0.1725265396070433
0.9682568990803648	0.6718249922835375	0.3087907113928723
0.6875500080000023	0.6666700239999983	0.0444899980000031
0.6895271704881951	0.1652340342592861	0.1802459529561662
0.6788605012663804	0.6643559367663181	0.3042678719712347
0.6457899810000001	0.0000000000000000	0.0444899980000031
0.6466724578314687	0.4978303025515333	0.1726480425668969
0.6357777342137781	0.0055516404149212	0.3088564214430112
0.3542099889999974	0.0000000000000000	0.0444899980000031
0.3569927486214171	0.4984321437964557	0.1810119911212532
0.3451534172874615	0.9971240301605186	0.3050522651490231
0.3124499919999977	0.3333300050000005	0.0444899980000031
0.3136444228262403	0.8308260022689685	0.1725999517335662
0.3017062359322350	0.3378876067902655	0.3090677196582986
0.0208800010000019	0.3333300050000005	0.0444899980000031
0.0228496947295307	0.8318104908089222	0.1801714979017197

0.0117507163867171	0.3311097007697226	0.3049840515381980
0.8542100189999999	0.0000000000000000	0.0444899980000031
0.8529734873062851	0.5025544660637542	0.1726096427941194
0.8644845184240868	0.9960624122524288	0.3087527623070032
0.8124499919999977	0.3333300050000005	0.0444899980000031
0.8104281934538534	0.8352445163366242	0.1800825369458906
0.8215121204551292	0.3364460427602012	0.3051808292044799
0.5208799839999969	0.3333300050000005	0.0444899980000031
0.5198596845224446	0.8345585571735384	0.1733292193652265
0.5310908096404987	0.3292720518734002	0.3086703797890480
0.4791199860000006	0.6666700239999983	0.0444899980000031
0.4769470538499754	0.1678229801657908	0.1802832346492560
0.4876324736061203	0.6700570728688626	0.3087229479990202
0.1875499929999975	0.6666700239999983	0.0444899980000031
0.1866018692755663	0.1690402634253819	0.1726447618387354
0.1962711898078710	0.6625162826144413	0.3083036691700212
0.1457899959999978	0.0000000000000000	0.0444899980000031
0.1439443970446767	0.5015030613791536	0.1799555406272006
0.1547244195536739	0.0030477268218745	0.3053068097027326
0.4990130070304439	0.6478425096793191	0.4483165381839172
0.3858194204669505	0.6163446750599484	0.4934615316302962
0.4201513240510470	0.8103775683929163	0.4661566488794557
0.3792618420431749	0.6649563372614917	0.4051691845621705
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9160376661235174	0.6806757766870201	0.2144713711435159

0.9170558532985419	0.1853442661344611	0.3450764310990363
0.9167399999999972	0.8334100249999992	0.0934000020000028
0.9165121566179860	0.3332210936763100	0.2222659599244171
0.9163837075847100	0.8338852691216269	0.3563878595234543
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9173058760732131	0.9868178198230090	0.2145837236254867
0.9161649945911977	0.4825109840920725	0.3451081741257201
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7484615407775582	0.6547396362973763	0.1376046885811862
0.7493119269225261	0.1517493204673161	0.2746617462362265
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7513662563060315	0.3455833087338697	0.1376134323325100
0.7508574719454585	0.8494298870635079	0.2738594297955015
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7500871581679298	0.0004654901895262	0.1284259251890577
0.7505993225493874	0.5001361742974235	0.2580557643273441
0.5833299760000017	0.5137699839999996	0.0795100030000029
0.5828356560845108	0.0134961165016727	0.2146578220488072
0.5859560388719345	0.5168416710122353	0.3448413735593047
0.5832600000000028	0.1665900050000033	0.0934000020000028
0.5829298065619579	0.6660551789756396	0.2228231172412716
0.5820984250115576	0.1663240683153851	0.3564103773692484
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5838246959071323	0.3194408289279170	0.2145190600372087
0.5850567138179691	0.8156007930069702	0.3452591914205537

0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4181650075525037	0.6786224928693725	0.1378830756774901
0.4167149784446589	0.1819155216227530	0.2740152687551295
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4151357454481229	0.9873057475856336	0.1378402303814280
0.4163257984724554	0.4846286422798701	0.2757045420074780
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4165967366473570	0.3334665906206493	0.1287272092660738
0.4171927671544993	0.8327622018186270	0.2595192217556178
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2508545692184660	0.6529086865877732	0.2147158098221503
0.2499794211276132	0.1481854538180860	0.3455816561576003
0.2500000000000000	0.5000000000000000	0.0934400040000014
0.2499932746099427	0.9998679573102215	0.2225010363335545
0.2471381041895062	0.4991418120333580	0.3558422927614558
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2495468887758855	0.3470336817102126	0.2147211753770651
0.2493793275401334	0.8511369708187072	0.3450073676183444
0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0849149423908088	0.0122271917323242	0.1377207758408603
0.0829462686411777	0.5158249580540675	0.2735988291025465
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0819820460397105	0.3210738225200198	0.1376191736714047
0.0825000590150677	0.8182115199030954	0.2742973490636281
0.0833299980000035	0.1666699949999995	0.0000000000000000

0.0835503648735587	0.6669638521309014	0.1284739729563201
0.0835240323057392	0.1670347270021447	0.2587024480595990

2. Transition structure of methane adsorption on α-Fe_2O_3(110) surface:

a = 13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c =19.23870 Å γ = 90.2605°

C	Fe	H	O
1	36	4	54

0.4049947406004380	0.6599885612677836	0.4262933294551784
0.9791200159999894	0.6666700239999983	0.0444899980000031
0.9796010642813791	0.1651001745807277	0.1726034293980777
0.9678965064630576	0.6738785140806588	0.3092947417458417
0.6875500079999970	0.6666700239999983	0.0444899980000031
0.6899813516953468	0.1648760701539999	0.1805206100477942
0.6729147251755360	0.6647219534935733	0.3028715122762395
0.6457899810000001	0.0000000000000000	0.0444899980000031
0.6471055091248468	0.4976366528343180	0.1724658449898732
0.6350576639838930	0.0048246522610434	0.3091874905084431
0.3542099889999973	0.0000000000000000	0.0444899980000031
0.3589956793362178	0.4990357661675107	0.1807710201107922
0.3447484744772137	0.9965713248946443	0.3043177129977915
0.3124499919999909	0.3333300050000005	0.0444899980000031
0.3144355116283769	0.8316775036783076	0.1723856478516537
0.3056757757154974	0.3360511194410853	0.3064486111597227

0.0208800010000014	0.3333300050000005	0.0444899980000031
0.0215549072164769	0.8323842886808307	0.1794327060261751
0.0108675384452361	0.3320476577095475	0.3052598194017878
0.8542100189999998	0.0000000000000000	0.0444899980000031
0.8527437575347655	0.5031909333071956	0.1726586515311688
0.8636445780165054	0.9974383908920984	0.3088988981171967
0.8124499919999977	0.3333300050000005	0.0444899980000031
0.8092213435681503	0.8350841570861489	0.1809624740540325
0.8207024499580026	0.3384646212146078	0.3053045348328876
0.5208799839999965	0.3333300050000005	0.0444899980000031
0.5201790957273711	0.8301896041997574	0.1759285969035446
0.5324202255397315	0.3305770386204331	0.3078006887252784
0.4791199860000004	0.6666700239999983	0.0444899980000031
0.4780418305350382	0.1661493380938747	0.1794776562673545
0.4763587719817582	0.6686764038054894	0.3222533622425871
0.1875499929999974	0.6666700239999983	0.0444899980000031
0.1863755076050180	0.1692960289785068	0.1721233590478291
0.1947486710495045	0.6685270979384883	0.3061859170248347
0.1457899959999978	0.0000000000000000	0.0444899980000031
0.1448344820746913	0.5016840026008855	0.1795599558391009
0.1535961077727302	0.0067650572249850	0.3047688819230666
0.4828317964912867	0.6918584799090972	0.4351488557515593
0.3919618608343221	0.5628395426074662	0.4628021019036375
0.3600537140581020	0.7606931589031358	0.4413609198998575
0.3393004370309302	0.5856040227899073	0.3804835121107604

0.9166700239999847	0.1804399939999968	0.0795100030000029
0.9163083111932100	0.6808292709309834	0.2149329021493452
0.9167959435501528	0.1868219433361995	0.3452535627575211
0.9167399999999972	0.8334100249999996	0.0934000020000028
0.9171122858071012	0.3349781870405902	0.2225745117723769
0.9177682310618948	0.8370728943868946	0.3566334538948852
0.9166700239999847	0.4862299859999981	0.0795100030000029
0.9168095569247215	0.9874888329346785	0.2147087251877548
0.9166453801316101	0.4840126223964709	0.3451977252965203
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7498359077740049	0.6544946604520033	0.1370771256433551
0.7496025394311090	0.1524503879506434	0.2748801059106698
0.7500000000000000	0.8471099730000023	0.0094599999999971
0.7521882954973144	0.3448345781818346	0.1378012481758867
0.7501518745942690	0.8496423302644992	0.2745656248650084
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7502111014630067	0.0001604249485714	0.1285286825841921
0.7499392150574176	0.5008073322105919	0.2582616699800703
0.5833299759999968	0.5137699839999996	0.0795100030000029
0.5826719853682375	0.0127891035933055	0.2148630328755249
0.5845959993963427	0.5168722270408623	0.3459457981065690
0.5832600000000028	0.1665900050000034	0.0934000020000028
0.5852011901159728	0.6656915054799478	0.2210362553331420
0.5817757666559590	0.1670269090520660	0.3560342117320795
0.5833299760000014	0.8195599909999985	0.0795100030000029

0.5846477396664467	0.3182386901404490	0.2139779269125577
0.5830204725534938	0.8165352968192180	0.3457100494521577
0.4166699949999993	0.1804399939999968	0.0094599999999971
0.4179804503390878	0.6791055904588402	0.1377454346517065
0.4162701460751248	0.1812631650257855	0.2734669164440727
0.4166699949999993	0.4862299859999981	0.0094599999999971
0.4150085791860706	0.9864712366877969	0.1382276355307499
0.4192804420325130	0.4815445376951350	0.2735882519716616
0.4166699949999995	0.8333299760000022	0.0000000000000000
0.4165978318845613	0.3325831017038208	0.1285288057611065
0.4159597226087709	0.8301298616433237	0.2611720848351238
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2510503742790768	0.6537154385357887	0.2143698425225027
0.2495798707723784	0.1534525266681077	0.3447299923361775
0.2500000000000000	0.5000000000000000	0.0934400040000014
0.2495582244301457	1.0004846229638626	0.2224388979469575
0.2652646856390743	0.5159538670360105	0.3564844337646556
0.2500000000000000	0.8471000190000031	0.0795100030000029
0.2496664304590270	0.3477737607307492	0.2147329019957808
0.2460353832890158	0.8551425815991250	0.3453291365298323
0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0846317338878461	0.0130482553940170	0.1377356701367335
0.0876705511413425	0.5151095324101606	0.2768684085392940
0.0833299980000035	0.8195599909999985	0.0094599999999971
0.0820743781291239	0.3217997752620234	0.1377820649349836

0.0824346404745876	0.8191641012335337	0.2734028399865971
0.0833299980000035	0.1666699949999996	0.0000000000000000
0.0834222344422926	0.6666300911011848	0.1288329208608592
0.0827513575943403	0.1686512771853829	0.2583516374831766

3. Intermediate structure of methane adsorption on α-Fe_2O_3(110) surface:

a = 13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605°

C	**Fe**	**H**	**O**
1	36	4	54

0.4196771615515436	0.6770220718581568	0.4286198330335378
0.9791200160000031	0.6666700239999983	0.0444899980000031
0.9794337372575003	0.1651391735004680	0.1724398848995963
0.9663473804715841	0.6736445754027759	0.3088854839358778
0.6875500080000023	0.6666700239999983	0.0444899980000031
0.6892899087846451	0.1651846175439266	0.1803256811733397
0.6727601820724309	0.6666013390082347	0.3022104956680702
0.6457899810000001	0.0000000000000000	0.0444899980000031
0.6476006340904520	0.4974650410824062	0.1723095093561546
0.6354022270891537	0.0085043022323789	0.3093498953164741
0.3542099889999974	0.0000000000000000	0.0444899980000031
0.3607550931463800	0.4990000688682077	0.1832932461211817
0.3458899742114009	-0.0091710102908227	0.3047939646993206
0.3124499919999977	0.3333300050000005	0.0444899980000031
0.3152112590751248	0.8310335865998383	0.1722999933377418

0.3063610321406972	0.3276848581984379	0.3056870581610723
0.0208800010000019	0.3333300050000005	0.0444899980000031
0.0207419818873808	0.8321949306266305	0.1786926560339046
0.0106511464254855	0.3318319471370514	0.3049990722746485
0.8542100189999999	0.0000000000000000	0.0444899980000031
0.8525985045440979	0.5030077976665722	0.1726872133015503
0.8635198384884765	0.9975703606614651	0.3085288671662654
0.8124499919999977	0.3333300050000005	0.0444899980000031
0.8088468461926732	0.8351169554136932	0.1806567683597429
0.8203740953564674	0.3391504489472799	0.3052908303573661
0.5208799839999969	0.3333300050000005	0.0444899980000031
0.5205145989126755	0.8295352353913472	0.1766700431606878
0.5320191616219572	0.3351049661464313	0.3083686648383295
0.4791199860000006	0.6666700239999983	0.0444899980000031
0.4778927818802145	0.1657559427256368	0.1796439847794287
0.4774059018165948	0.6747870757770618	0.3291222348700371
0.1875499929999975	0.6666700239999983	0.0444899980000031
0.1865200008525266	0.1674393599336067	0.1721090956932413
0.1900599097738672	0.6697842661692507	0.3038786180567620
0.1457899959999978	0.0000000000000000	0.0444899980000031
0.1454476809065211	0.5004491905724021	0.1781170833551874
0.1539296760907751	0.0060239912955012	0.3049743283906465
0.4795403225210823	0.7300377530812051	0.4588567297657959
0.4101593099199695	0.5556101729259877	0.4471001862362436
0.3524547167553759	0.7459562484347592	0.4347808697776268

0.2899810900854782	0.5434000859943855	0.3948612500330298
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9161897878630770	0.6810609615201758	0.2144820148303146
0.9165576643872742	0.1869561687240026	0.3450201424196368
0.9167399999999972	0.8334100249999992	0.0934000020000028
0.9170953169646583	0.3344988293502995	0.2224870881584823
0.9182032328664462	0.8377718450788807	0.3564356369103727
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9170741957782869	0.9876597610848579	0.2144709578483869
0.9168653163255535	0.4838774911193867	0.3453913280909382
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7507021408056004	0.6541562337299356	0.1363585983918120
0.7489584194805028	0.1537422740851928	0.2749524900377092
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7521389622127068	0.3444190650592769	0.1376969082689650
0.7513696842341540	0.8508075682246046	0.2737803960523204
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7500661063114966	0.0006654952092949	0.1284130382718608
0.7509214420311650	0.5015745360907155	0.2576863579181776
0.5833299760000017	0.5137699839999996	0.0795100030000029
0.5825590432004016	0.0138187130627407	0.2149207518677737
0.5872095039261455	0.5183982384627510	0.3459809325988645
0.5832600000000028	0.1665900050000033	0.0934000020000028
0.5876481596441033	0.6669993099882779	0.2195780950129053
0.5793451061566237	0.1692214552255673	0.3559076814732839

0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5834705123849085	0.3197732893222282	0.2142072816453792
0.5867522606188601	0.8203392841719032	0.3462101014305421
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4182304957479744	0.6777334037614399	0.1382529905805476
0.4148246345663698	0.1793220099961953	0.2729205724265049
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4148737179037381	0.9861770158104661	0.1382074750689787
0.4145337894865672	0.4817735368425136	0.2797741021609463
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4163123105320227	0.3332779740124771	0.1293196575764478
0.4171855663671490	0.8292280418802255	0.2609656846876945
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2515364291460249	0.6521540490332328	0.2149344346488036
0.2509174882130841	0.1477241727122827	0.3459472070426868
0.2500000000000000	0.5000000000000000	0.0934400040000014
0.2493071348481186	0.9984116253701517	0.2229166649942494
0.2442677435317006	0.4990981422268125	0.3606619591085769
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2496958214633771	0.3460843350757979	0.2152875687110510
0.2450269338235365	0.8489770292542971	0.3452984926084173
0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0847196567329410	0.0127087739824328	0.1377778331047338
0.0857565316016434	0.5146971338946253	0.2742472987602439
0.0833299980000035	0.8195599909999984	0.0094599999999971

0.0823966347705759	0.3204782723468464	0.1376164459222506
0.0819468431921133	0.8185956110584932	0.2729523395392879
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0837323187592281	0.6667731727282354	0.1286553838982478
0.0833784445179094	0.1679201941396134	0.2589465031502531

4. Initial structure of methane adsorption on α-Ir/Fe_2O_3(110) surface:

a =13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605°

C	Fe	H	Ir	O
1	35	4	1	54

0.4432874413167721	0.3663297506046145	0.4468208963220686
0.9879000190000014	0.6708599930000005	0.0471200010000032
0.9795149250474876	0.1687417803521988	0.1753349464501166
0.9670413810997036	0.6661464456960814	0.3110856170490068
0.6955100300000012	0.6614500279999973	0.0453899990000011
0.6920411920289022	0.1649739269053778	0.1841374792201645
0.6835931813085151	0.6594678945897893	0.3052818328631142
0.6546700000000030	0.0039900000000017	0.0470100009999967
0.6448844927107914	0.4985039466934674	0.1730977550193172
0.6418963410690218	0.9972671293547218	0.3077041740793985
0.3623999949999970	0.9950399989999994	0.0452999990000009
0.3531514090689228	0.4995242274921619	0.1810135894264704
0.3416027697549770	0.9908877089505728	0.3060938240439815

0.3212400079999966	0.3376100059999985	0.0470600020000020
0.3104628270330459	0.8309154717473740	0.1712884504897885
0.2988749349996687	0.3400766303180908	0.3110948172912920
0.0288100000000000	0.3282800019999996	0.0453100020000008
0.0232503309163944	0.8346780420143485	0.1835986851321249
0.0200010761548843	0.3274982152273664	0.3177077111130308
0.8452699779999975	0.9957699779999984	0.0471200010000032
0.8554377939663138	0.4998976302458519	0.1722408276533378
0.8677676468881114	0.9952815528740488	0.3114155917379631
0.8043900130000026	0.3382999900000030	0.0453199999999967
0.8142100147809971	0.8323720474727340	0.1815942984635566
0.8278299195210834	0.3374905356220350	0.3058490051216041
0.5121799710000019	0.3290899989999971	0.0473399979999982
0.5224188383384393	0.8335298544921222	0.1713281126014455
0.4709595725829985	0.6716853913040026	0.0453841558730019
0.4802881940414542	0.1638434509625623	0.1797721690577396
0.4910442474552462	0.6772598484946141	0.3059904042189420
0.1777216767870016	0.6620344904570032	0.0471823193590026
0.1874988651278499	0.1672636041534482	0.1725593372573828
0.1960260141182355	0.6647972547510299	0.3107167840293900
0.1370828061009988	0.0052962692289995	0.0456013446709989
0.1415106592535239	0.4996205243432067	0.1847097061945555
0.1520419926882635	0.0068675426296816	0.3067029135720283
0.5153417150853777	0.4145285490572891	0.4591927009808452
0.4458719211780744	0.2820335728821249	0.4005777443982930

0.4183313787001206	0.2830729652270420	0.4868185000854807
0.3879370552840824	0.4561088316192317	0.4372128750947508
0.5175505509883852	0.3255467423503747	0.3170113484135825
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9166266978650036	0.6791960667705499	0.2157757631359803
0.9142679639678684	0.1835003996138007	0.3506000705921856
0.9168900250000007	0.8334699870000009	0.0939000030000017
0.9146065564342910	0.3319715700105239	0.2223694294429398
0.9214311325252458	0.8349268204731195	0.3582369575039616
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9175249332347338	0.9859861753210708	0.2162930865658493
0.9076599464402995	0.4911546827772749	0.3493013713720012
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7493732259194469	0.6534927265965289	0.1394266880512775
0.7508143452289781	0.1504439567516739	0.2753061888259365
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7464364787895515	0.3453228700116309	0.1385652582977775
0.7530434746026962	0.8470263270901125	0.2756557371920659
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7501515294324117	0.9990071399062540	0.1308519831181141
0.7481927604145724	0.4956691091326159	0.2584948855930520
0.5833299760000017	0.5137699839999996	0.0795100030000029
0.5845326048605468	0.0122381662398428	0.2159226294061138
0.5831331015416878	0.5176719615533620	0.3482723772170963
0.5831099749999993	0.1653999979999980	0.0930399969999982

0.5844369372649973	0.6679255201106932	0.2240533691920018
0.5898051466148100	0.1616868110747221	0.3589259576503889
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5774725742759180	0.3209820908707395	0.2211449086126714
0.5883577362832086	0.8122620348381361	0.3476015786738835
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4170036938392474	0.6791488870896261	0.1395459213860401
0.4186349841399728	0.1744422580094393	0.2733839087052689
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4171458549501073	0.9848920602478667	0.1389287392501639
0.4175830158429136	0.4875119565413810	0.2756050694075512
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4168408037460419	0.3326796507303129	0.1308495701893380
0.4176323970647737	0.8338831503471615	0.2611557219741767
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2507876637471111	0.6530530623265289	0.2168343940382843
0.2515197897978086	0.1489458472053971	0.3472452374279174
0.2497400049999996	0.4999499919999977	0.0940900000000013
0.2512731554377368	-0.0005185480521038	0.2234734909109067
0.2490884868544311	0.5022969438418818	0.3590884199791913
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2493810077582228	0.3472830973011189	0.2165966823409682
0.2490845974361455	0.8514685245526917	0.3478805175888867
0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0836318273407332	0.0119579671936188	0.1384188471466663

0.0832769335398198	0.5219054340356911	0.2778844475715895
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0836294299681566	0.3220884379037729	0.1387422887898951
0.0841509901754966	0.8206816193882052	0.2751161582945150
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0833955993406985	0.6665897790313898	0.1309790618689834
0.0849588939906480	0.1622892720361174	0.2560844635431927

5. Transition structure of methane adsorption on α-Ir/Fe_2O_3(110) surface:

a =13.66150 Å α = 90.0000°

b =8.56060 Å β = 90.0000°

c =19.23870 Å γ = 90.2605°

C	Fe	H	Ir	O
1	35	4	1	54

0.4539004539786816	0.3187466832150913	0.4275734791050578
0.9879000190000012	0.6708599930000005	0.0471200010000032
0.9792232417917973	0.1688131185861104	0.1752609852791309
0.9673550475250277	0.6656971799429171	0.3110295661588516
0.6955100300000012	0.6614500279999974	0.0453899990000011
0.6908697871112689	0.1676581822629775	0.1836481057540153
0.6829954982382919	0.6588806205010634	0.3051945929026711
0.6546700000000025	0.0039900000000017	0.0470100009999967
0.6443031295796222	0.4982283534928921	0.1728126956467723
0.6430226603739686	0.9970904250873592	0.3072073206841134
0.3623999949999970	0.9950399989999995	0.0452999990000009
0.3530676872100582	0.4996919420825748	0.1810159692430273

0.3409557724069477	0.9912720814513345	0.3062376386786535
0.3212400079999767	0.3376100059999985	0.0470600020000020
0.3106146110815778	0.8315166879398395	0.1713605472208725
0.2985007606257157	0.3397144383765686	0.3116053833470539
0.0288100000000000	0.3282800019999999	0.0453100020000008
0.0230750395619995	0.8348014569024405	0.1834977930630751
0.0198736349577048	0.3271533265215080	0.3178108408211437
0.8452699779999970	0.9957699779999990	0.0471200010000032
0.8553448164687643	0.5003178254737259	0.1721568878106697
0.8679341561726124	0.9947375645496257	0.3115048361561482
0.8043900130000025	0.3382999900000032	0.0453199999999967
0.8139264340464416	0.8327872637258381	0.1814017038407498
0.8274332182911850	0.3373355552343764	0.3057703697716744
0.5121799710000019	0.3290899989999974	0.0473399979999982
0.5222498750778932	0.8344166092179475	0.1712055789755418
0.4709597585461010	0.6716829836133443	0.0453823088183256
0.4807611698362703	0.1662339471896889	0.1806234305213962
0.4910659957823867	0.6778168525264424	0.3060160538804348
0.1777209293261136	0.6620369369205582	0.0471812889772210
0.1874526677303236	0.1675259799967317	0.1725443627891112
0.1963990478138355	0.6649076412977719	0.3108996192709804
0.1370815585005615	0.0052979273494529	0.0456007474838742
0.1415918360446585	0.4997163993202833	0.1848057968429511
0.1512382478922412	0.0069782014112472	0.3066383438760352
0.5013877598730377	0.3572598594828380	0.4707826329883332

0.5227911383506380	0.2263682531735180	0.4040736807244725
0.4017991657513062	0.2269217264212378	0.4435224574705733
0.4105217385938797	0.4228312576623565	0.4142176028054596
0.5171679725864412	0.3270235191086687	0.3177940585433849
0.9166700239999584	0.1804399939999968	0.0795100030000029
0.9164226495919229	0.6794340512729586	0.2158896451782690
0.9137386517958230	0.1833171674876156	0.3505180999054207
0.9168900250000007	0.8334699870000009	0.0939000030000017
0.9141646961032681	0.3318270360633222	0.2223748212819516
0.9217786637121659	0.8345146626375259	0.3582879624247793
0.9166700239999584	0.4862299859999981	0.0795100030000029
0.9172089653163922	0.9860119481567027	0.2162818587125562
0.9081261841541706	0.4903974310201610	0.3491191628799563
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7492727224728617	0.6539791376967576	0.1394401969263733
0.7496264382814716	0.1504298902625888	0.2754856446528500
0.7500000000000000	0.8471099730000023	0.0094599999999971
0.7474800955697832	0.3463492773381475	0.1383746134340462
0.7528313363374249	0.8472885301235291	0.2759773864093878
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7496152404087043	0.9997148379484020	0.1309889544449421
0.7481767269887384	0.4962053287799140	0.2588884054158893
0.5833299759999968	0.5137699839999996	0.0795100030000029
0.5841045461971487	0.0123980725710404	0.2166184550034513
0.5825210479992912	0.5202136310325605	0.3490172195778797

0.5831099749999993	0.1653999979999980	0.0930399969999982
0.5843036236033207	0.6686984565767740	0.2241690437660389
0.5930934982954779	0.1631653550705306	0.3630916809507679
0.5833299760000014	0.8195599909999985	0.0795100030000029
0.5792862150936923	0.3213403205267824	0.2180397993364685
0.5880497174162291	0.8151346280500225	0.3472852182887106
0.4166699949999993	0.1804399939999968	0.0094599999999971
0.4171243250671116	0.6794108066770974	0.1397185711626910
0.4196885385021569	0.1747576304033700	0.2752547606264915
0.4166699949999993	0.4862299859999981	0.0094599999999971
0.4173170770224687	0.9860220395244623	0.1392377058431237
0.4178939272401520	0.4864872520467596	0.2761863920629967
0.4166699949999995	0.8333299760000022	0.0000000000000000
0.4162421463861487	0.3326336102600622	0.1308776749019013
0.4170429488709484	0.8338392621940788	0.2614501668561897
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2509673059476648	0.6531739672053039	0.2168993571284741
0.2499974727115743	0.1491866824055418	0.3471231545938770
0.2497400049999996	0.4999499919999977	0.0940900000000013
0.2512432061957643	0.0000131735503943	0.2235311619894619
0.2504496072121805	0.5034354976472184	0.3594486014937087
0.2500000000000000	0.8471000190000031	0.0795100030000029
0.2496695099308122	0.3472745067518801	0.2168457202554649
0.2486741207994577	0.8520655834064353	0.3480275395712161
0.0833299980000035	0.5137699839999996	0.0094599999999971

0.0836227298146886	0.0120441141500814	0.1384230708001033
0.0838819874539144	0.5215457609095384	0.2781718201729811
0.0833299980000035	0.8195599909999985	0.0094599999999971
0.0836394384851434	0.3222581158862265	0.1387746997674840
0.0840558586100947	0.8203818953615279	0.2749091673365304
0.0833299980000035	0.1666699949999996	0.0000000000000000
0.0833720468822668	0.6665818867892663	0.1310446210697994
0.0844391548431053	0.1625495700484638	0.2558798928713319

6. Intermediate structure of methane adsorption on α-Ir/Fe_2O_3(110) surface:

a =13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c =19.23870 Å γ = 90.2605°

C	Fe	H	Ir	O
1	35	4	1	54

0.4433441242658865	0.3408586675258102	0.4180283234817023
0.9879000190000014	0.6708599930000005	0.0471200010000032
0.9790917696881959	0.1697449600752632	0.1753014348512432
0.9661003821520042	0.6664943797316968	0.3108304307118652
0.6955100300000012	0.6614500279999973	0.0453899990000011
0.6899378592801715	0.1704615253161215	0.1823929696497364
0.6811330190892130	0.6571249384672510	0.3058118203985537
0.6546700000000030	0.0039900000000017	0.0470100009999967
0.6432718068019093	0.4977436124682833	0.1730496299022507
0.6462908722809652	0.9941776521026799	0.3042889609108446
0.3623999949999970	0.9950399989999994	0.0452999990000009

0.3520496991208874	0.4998193442260372	0.1812002685027340
0.3396106247468464	0.9942506360817729	0.3065390487811711
0.3212400079999966	0.3376100059999985	0.0470600020000020
0.3105452548591560	0.8328848313371934	0.1716065670187803
0.2971408669693070	0.3441116720832676	0.3144297831216925
0.0288100000000000	0.3282800019999996	0.0453100020000008
0.0228163134533180	0.8356795325970146	0.1831845264625387
0.0196929457081115	0.3291654543620051	0.3178076394424279
0.8452699779999975	0.9957699779999984	0.0471200010000032
0.8551170095311745	0.5011322615388384	0.1718852520601988
0.8686068068083994	0.9958815237386929	0.3113435994995591
0.8043900130000026	0.3382999900000030	0.0453199999999967
0.8136903501377675	0.8330397348207160	0.1809568230488353
0.8271272887912637	0.3380127142052160	0.3056304786090417
0.5121799710000019	0.3290899989999971	0.0473399979999982
0.5215761797132842	0.8343821883707035	0.1709756060475201
0.4709599910000009	0.6716799739999999	0.0453800000000015
0.4812673163443343	0.1686862532893804	0.1821499849613316
0.4899245220921123	0.6817848287698087	0.3071281557726149
0.1777199949999968	0.6620399950000007	0.0471800010000010
0.1876397965354659	0.1690240137672298	0.1726627378786304
0.1938084542873514	0.6690048180466154	0.3102316277219200
0.1370799990000009	0.0052999999999983	0.0456000009999968
0.1412743285534383	0.5002941002004218	0.1848420046891255
0.1501679758273327	0.0096044216538420	0.3069131747224214

0.5013067297640228	0.3732929058087384	0.4552538776184463
0.5682390144826768	0.1390598150060085	0.4103856029185921
0.4108385042178391	0.2271888326766085	0.4327805426550534
0.3860585853008176	0.4310421722787677	0.4218145925272489
0.5105962044797271	0.3330201569822693	0.3217260023165369
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9158408518521256	0.6803050483159837	0.2156917560971483
0.9136620579143391	0.1844646268577044	0.3505445645284854
0.9168900250000007	0.8334699870000009	0.0939000030000017
0.9133938565183775	0.3323598080499423	0.2223677593370074
0.9211526158287386	0.8353330376896104	0.3585380501798415
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9168779396370397	0.9867785505950529	0.2161432940079427
0.9071718031337052	0.4913673308734170	0.3492820621079150
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7487283242741982	0.6543974081799503	0.1396000900326617
0.7487624139592363	0.1505231498369772	0.2758086112571818
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7483845001931456	0.3479194236022392	0.1381413505867183
0.7526599125286351	0.8455550330824484	0.2756634300809660
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7494697673597750	0.0003771127512075	0.1309656643779012
0.7470946033345048	0.4963964523176719	0.2596147104470051
0.5833299760000017	0.5137699839999996	0.0795100030000029
0.5841648565042190	0.0112142804160814	0.2162929712951046

0.5793324749567567	0.5245867791771158	0.3512766342633800
0.5831099749999993	0.1653999979999980	0.0930399969999982
0.5831395567589515	0.6687169982411415	0.2251503633428600
0.5945986908745261	0.1679977922496169	0.3648048415363360
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5817526696860756	0.3189322347183973	0.2159345237523130
0.5877174521997400	0.8210983564879564	0.3478818398495162
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4168277161728253	0.6795583806054193	0.1399904015150164
0.4204819346764146	0.1751112623881217	0.2771896111594343
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4174316173344987	0.9872792904497539	0.1396058308624390
0.4158924345358605	0.4891024673942870	0.2778093540178415
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4159793018668866	0.3330721333602526	0.1312894243486877
0.4158445493372462	0.8357577229420536	0.2620478257367571
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2504912639750611	0.6544481306456535	0.2169442157521644
0.2479133919418693	0.1515581368375910	0.3472793188305884
0.2497400049999996	0.4999499919999977	0.0940900000000013
0.2506512395878171	0.0014376060195805	0.2236652884879057
0.2423264914333685	0.5055295388564843	0.3596838220053762
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2496443391254720	0.3482879179010165	0.2179843625475987
0.2475465753575125	0.8544785268974403	0.3482683770687576

0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0836371553868642	0.0128471355810842	0.1384471264562122
0.0813905119547137	0.5237297369420970	0.2767694410326285
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0836961101883508	0.3228568495555851	0.1386842344562008
0.0830530622937821	0.8224317218751482	0.2749582041803966
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0832600776035767	0.6671459131005431	0.1309637371718034
0.0834488476332483	0.1642953609825137	0.2557255171196485

7. Initial structure of methane adsorption on α-Ir/Fe_2O_3(110)-O_V surface:

a =13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605°

C	Fe	H	Ir	O
1	35	4	1	53

0.6150249318240115	0.4090565074098663	0.4148380167151556
0.9879386295190002	0.6708852831529981	0.0471818204550019
0.9794819037748046	0.1651149046320610	0.1726391480020888
0.9692544862792546	0.6716650649179725	0.3105504424517636
0.6955655656550022	0.6614624020240001	0.0453409369020008
0.6890558028671980	0.1681019330323777	0.1873636997420036
0.6953659144953914	0.6641249954494867	0.3052941778992493
0.6546598067689970	0.0039537136630017	0.0471157021409994
0.6436828263396904	0.4950887594882640	0.1730686368193604
0.6312393735678283	0.9856778215733585	0.3110889673306202

0.3623605094620004	0.9949854423459996	0.0453463047469995
0.3545977564958109	0.4975285890868630	0.1827098476624197
0.3443831446607434	0.9929270764830191	0.3075894816594308
0.3213507213540012	0.3377258383129984	0.0471271640720019
0.3115774223767923	0.8316715590535410	0.1715133137915415
0.3042891070243519	0.3393401515717769	0.3156578104774105
0.0286894169090033	0.3281823687930014	0.0452874214970009
0.0220499517831633	0.8340231164120906	0.1829750432551153
0.0127915279527717	0.3307705278458747	0.3079006013758941
0.8453391402499975	0.9959138295349987	0.0472253298010017
0.8543156933190194	0.5014888217949873	0.1719716829075727
0.8639979759110756	0.9947038095048434	0.3112660300259839
0.8045265554040029	0.3381685050470011	0.0452105561310034
0.8114571480371663	0.8354980351833777	0.1816808607994489
0.8230194358412982	0.3335357731744854	0.3061700809927556
0.5123228832730007	0.3294095921010012	0.0474033937359977
0.5227432216651178	0.8334165502610907	0.1705811175912148
0.4712415014099989	0.6715918206569995	0.0454063771489999
0.4827939304576302	0.1667749013962050	0.1787220412527428
0.4912332399982256	0.6712080046972122	0.2994151203277879
0.1787305590139994	0.6625370348399997	0.0471102783410018
0.1900440393500246	0.1694697949189139	0.1726081161075059
0.1982000721424968	0.6622694496195850	0.3112379850377774
0.1379506333559988	0.0050515697120019	0.0452295293950016
0.1453102102661609	0.4995676421259814	0.1830208361917487

0.1548449334725559	0.0043470547142826	0.3063848396899320
0.5343084168795861	0.4346811615980010	0.3959795669610820
0.6395379907209021	0.5284618573999834	0.4274720705222175
0.6056155281298581	0.3368277523058231	0.4614075426182835
0.6660600192815945	0.3516813880936700	0.3791453114907378
0.5022296038311981	0.3065322021650129	0.3244532895292675
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9156326853836060	0.6800707226316561	0.2163856859498373
0.9166144517328980	0.1845291595502848	0.3486218311030220
0.9168837479650023	0.8333063657279993	0.0939248907709995
0.9163771919669721	0.3291872762292039	0.2242422083773656
0.9146174573299136	0.8308712065502580	0.3585935845806001
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9169591720997108	0.9877558947746615	0.2166208686588480
0.9188063857640932	0.4830555163709983	0.3467199173482642
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7499417986793747	0.6531144806853634	0.1395550260766723
0.7400310400984841	0.1554022715677042	0.2840641048921899
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7499956977121379	0.3436573358149357	0.1396657468348600
0.7517825930573696	0.8635398634266181	0.2738224886553629
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7495313247612394	0.0029638257510161	0.1312206535133542
0.7497935330324828	0.4904125477844862	0.2596123443945703
0.5839357377439995	0.5144648866819992	0.0784007022329973

0.5834366855504139	0.0096907181864957	0.2165867475372012
0.5833969934650014	0.1659377339019983	0.0936622551799999
0.5824793444903255	0.6626650887568822	0.2219253868087470
0.5530873135610612	0.1173963756114116	0.3629894998436739
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5808865061571017	0.3195108871878705	0.2170245734022719
0.5891512476795436	0.7790529790991688	0.3506403095045809
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4158689553268634	0.6786596101303528	0.1392591110784344
0.4123074071868304	0.1768261600618553	0.2665701393186284
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4171819006839774	0.9851660780499834	0.1386469354650990
0.4203510427507645	0.4871038541574923	0.2759632377286187
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4165481845135208	0.3339148585974339	0.1299500574223570
0.4183576241381298	0.8354053281315557	0.2611020866795220
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2516103457985784	0.6538128544230489	0.2171082546990895
0.2507986439530767	0.1473231732699102	0.3474995643187715
0.2497689701489989	0.5001631872089973	0.0942163245230034
0.2502902387497924	0.9988193821765641	0.2239738903621779
0.2510634217082265	0.5035767181644080	0.3603423741172962
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2503135985882402	0.3481433232020303	0.2180130509519976
0.2493924971290246	0.8516467128055608	0.3475082910596010

0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0841400257704102	0.0127700805367156	0.1392206922705105
0.0843341573731559	0.5185270445592488	0.2768302679914590
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0838579557374566	0.3209062984507636	0.1391870905999065
0.0821762656302928	0.8198695874769769	0.2762158805238867
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0834777126527994	0.6667015686822509	0.1311313383931647
0.0833309204326576	0.1668630357026933	0.2593588580392938

8. Transition structure of methane adsorption on α-Ir/Fe_2O_3(110)-O_V surface:

a = 13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605°

C	**Fe**	**H**	**Ir**	**O**
1	35	4	1	53

0.4832051740250023	0.3766144622169989	0.4297131810370018
0.9879528827840005	0.6708328507570016	0.0471576645820022
0.9788276116269969	0.1658619843620031	0.1728912685819992
0.9697958637759996	0.6720991700070016	0.3103792717829990
0.6956773925030006	0.6616612605769987	0.0453522449150014
0.6873661247940035	0.1687285530019977	0.1830050563949968
0.6897675516799993	0.6619799914699982	0.3089757757449973
0.6545283940340028	0.0043413473379985	0.0473678770219976
0.6440908655849995	0.5000274061910019	0.1733789905790033
0.6390851575339980	0.9956824695830022	0.3101399674180030

0.3621910495860021	0.9948601625480009	0.0453097730620016
0.3551792712899982	0.5004171907759982	0.1816255911190012
0.3425411625700008	0.9920002709569999	0.3063784192460020
0.3211596665019982	0.3376005973680023	0.0472076275099980
0.3113885960620024	0.8321563817919966	0.1718489598739978
0.3038661728599976	0.3328344520789983	0.3112389730479990
0.0287215027509973	0.3282102758129994	0.0452997425470016
0.0219522752420005	0.8338070376530027	0.1823178301189969
0.0110788336300018	0.3314599051469997	0.3078846144410008
0.8454573653329973	0.9959083394640018	0.0471888519670003
0.8546222803289965	0.5023923218849973	0.1717500527379983
0.8664987336619987	0.9953007591469998	0.3107369530800028
0.8044725748190018	0.3382701221210027	0.0453201122230027
0.8110019669850033	0.8353583746130013	0.1829140100210012
0.8203161708349995	0.3344299973850013	0.3056575306439981
0.5119769658469977	0.3295500607979989	0.0472528449679999
0.5218580393799996	0.8372153627529997	0.1711269096959995
0.4712905733769972	0.6717277508859993	0.0453619542290014
0.4780359299990025	0.1694607217039987	0.1844639039300020
0.4940872280039983	0.6710719409090018	0.3007445479070014
0.1787111151660028	0.6625718241679976	0.0471282144609972
0.1886505160209992	0.1683365346680006	0.1720693055460032
0.1997887310010000	0.6591868893389972	0.3114899804149971
0.1379521757380004	0.0049926750490030	0.0451991862580030
0.1450835407590034	0.4996135921940024	0.1830234973599971

0.1528975206789980	0.0024411703439995	0.3063247478430000
0.4739142033790031	0.2856789129190034	0.4705310772099978
0.5321316273950032	0.2519222064230036	0.4024135282040007
0.4094755076320027	0.4256151318620027	0.4231846653310001
0.5338914601249982	0.4645268861919973	0.4508697086910018
0.5262172589870033	0.3442908323480012	0.3185164034980019
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9156548985899988	0.6803254629939985	0.2163416829870002
0.9143697435520011	0.1867589535079972	0.3489315158539981
0.9164983921509986	0.8329117245779969	0.0935110368779988
0.9164177716169988	0.3314533854630000	0.2239754560630018
0.9192328745499978	0.8343483165090007	0.3587508227840033
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9174059533510004	0.9866820781650034	0.2159060509209993
0.9181160388359970	0.4844434663390018	0.3459980245890009
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7501052078440011	0.6546100629349993	0.1396294381500027
0.7484084172929997	0.1538742372069990	0.2741967918889969
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7495329929690016	0.3469613422560016	0.1392353821480015
0.7528073336760031	0.8606365840079988	0.2761459683219982
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7490074689039972	0.0007375385640032	0.1308991353419984
0.7480488159100034	0.4943241751529968	0.2603484383350008
0.5837998191019977	0.5139018858349971	0.0790589590280035

0.5819202767239986	0.0139796769810019	0.2186679798009976
0.5833077958239983	0.1678081312290018	0.0950189673090023
0.5829873480039964	0.6679783469350014	0.2214526474559975
0.5987446968799972	0.1674221535820024	0.3647703453479991
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5790023645749969	0.3229638219609967	0.2166765610540011
0.5881049793569986	0.7961430545789980	0.3497759528260005
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4159667946100001	0.6807225230310010	0.1386539373269997
0.4127530056900000	0.1768542469949992	0.2757316761650017
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4165873919439989	0.9884184796249968	0.1395443414539983
0.4201532798560024	0.4899720623850001	0.2743092104879992
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4158133476909995	0.3330555864380003	0.1305651340390028
0.4171082447060002	0.8340913152440024	0.2606674804929980
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2513968437759999	0.6528611893640033	0.2167245434919991
0.2477432780460020	0.1469063557949966	0.3473606943240028
0.2496796483849977	0.4998791832390026	0.0940518276419979
0.2487475459469977	0.9984489267850023	0.2236724085109998
0.2558955961290010	0.4989913343479984	0.3584811016350002
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2503490902809986	0.3464956811950017	0.2167474642909966
0.2473771305210022	0.8502187810150020	0.3469947348775216

0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0836293620480006	0.0130695183519975	0.1387828754929998
0.0854922778040006	0.5176963614609988	0.2774444650380019
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0834351206990007	0.3212954885430008	0.1392030944129985
0.0823455113339975	0.8184945449430003	0.2747417216160031
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0834975646500027	0.6662626738890012	0.1308766248009974
0.0816527305720030	0.1664124384830004	0.2592730129739991

9. Intermediate structure of methane adsorption on α-Ir/Fe_2O_3(110)-O_V surface:

a = 13.66150 Å α = 90.0000°

b = 8.56060 Å β = 90.0000°

c = 19.23870 Å γ = 90.2605

C	Fe	H	Ir	O
1	35	4	1	53

0.4737308030396034	0.4092186287273420	0.4223475271145464
0.9879500269999966	0.6708300109999996	0.0471599999999981
0.9790318911922303	0.1657687471136021	0.1728681089241524
0.9691352181703494	0.6716281156690872	0.3103582727089355
0.6956800219999977	0.6616600159999990	0.0453499999999991
0.6867957408147664	0.1704041546739502	0.1825374027535192
0.6889048781936545	0.6603952691546484	0.3090710747771734
0.6545299889999967	0.0043399999999991	0.0473700020000010
0.6429345790726867	0.4987471758226115	0.1738846878993770
0.6416378081512408	0.9912105071619709	0.3068792905958650

0.3621900079999989	0.9948599929999986	0.0453100020000008
0.3530593001955762	0.5003749286440805	0.1810494693549120
0.3430443725006688	0.9939863388889859	0.3059362737213654
0.3211599890000016	0.3375999929999978	0.0472099999999998
0.3113114300533429	0.8328586729007035	0.1719396923208108
0.3050348773815197	0.3366123372541880	0.3136890366148712
0.0287200010000035	0.3282099959999982	0.0452999990000009
0.0225060536377336	0.8340218515872850	0.1826636743091397
0.0109645300827913	0.3313492900143154	0.3079872798379044
0.8454599980000026	0.9959099889999976	0.0471899989999969
0.8543965448446245	0.5023305426322487	0.1717514650186672
0.8669460053693746	0.9947567282409375	0.3106436500542935
0.8044700029999987	0.3382700089999986	0.0453199999999967
0.8116528729240253	0.8348101286107685	0.1818108853151103
0.8201638983517315	0.3343895953967781	0.3056894786132939
0.5119799969999974	0.3295499979999974	0.0472499990000017
0.5208167712074548	0.8360631840293521	0.1710216955527700
0.4712899920000027	0.6717299820000022	0.0453599989999987
0.4790907654834394	0.1712856894879995	0.1842727797943235
0.4937170555243178	0.6710975847325269	0.3016607222049557
0.1787099989999987	0.6625700000000023	0.0471300000000028
0.1891728138867000	0.1695983012468405	0.1722156051103365
0.1984482952181814	0.6617207239646616	0.3112442051107981
0.1379500030000003	0.0049899999999994	0.0452000009999978
0.1443976366633153	0.4996851883711355	0.1834672737732802

0.1537041991704261	0.0040066374682764	0.3066272324519522
0.4528278040557366	0.3055223298700773	0.4535574048949079
0.5676791262675092	0.1495548673437597	0.4121150433101242
0.4128188418943949	0.4931104554998724	0.4261927287193880
0.5391354133780593	0.4622498592965280	0.4473038166457601
0.5150270451895640	0.3526997610445019	0.3222885230638893
0.9166700239999983	0.1804399939999968	0.0795100030000029
0.9155441170096995	0.6803125619792508	0.2162408668784825
0.9138258348342649	0.1863219290531570	0.3490484725903455
0.9164999719999969	0.8329100010000019	0.0935100020000021
0.9155305781396716	0.3303701680990880	0.2241429714729460
0.9179426989391168	0.8332721212260042	0.3589851509911363
0.9166700239999983	0.4862299859999979	0.0795100030000029
0.9172229979148131	0.9868428293855176	0.2159059158132998
0.9173615076132831	0.4839135703140924	0.3461718823724759
0.7500000000000000	0.1528899970000026	0.0094599999999971
0.7497576264968507	0.6540771790987979	0.1396847796636369
0.7454316334244597	0.1531434044696732	0.2765116169450462
0.7500000000000000	0.8471099730000020	0.0094599999999971
0.7498231190000442	0.3470593552213251	0.1392460857566040
0.7531373231709587	0.8589587885459692	0.2753398574062426
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.7490756599306637	0.0013783686737236	0.1310319352367447
0.7478166634110575	0.4937528469631156	0.2604622909902483
0.5838000179999980	0.5138999819999981	0.0790600030000022

0.5822905328803452	0.0123569201430464	0.2180968362947123
0.5833100079999980	0.1678099929999988	0.0950200039999984
0.5824158161071510	0.6675068656230148	0.2219931021086135
0.5925675919608668	0.1713183059614834	0.3653987965279377
0.5833299760000017	0.8195599909999984	0.0795100030000029
0.5802954501386479	0.3201939526003033	0.2168107248640372
0.5890109470607978	0.8012332581450636	0.3495911802802815
0.4166699949999995	0.1804399939999968	0.0094599999999971
0.4154576116294045	0.6810591263662853	0.1385864219132928
0.4143647222588076	0.1779516687084045	0.2753277873303227
0.4166699949999995	0.4862299859999979	0.0094599999999971
0.4168046079648525	0.9891119199054343	0.1395239616817444
0.4166890904239089	0.4943623155225077	0.2733274912254061
0.4166699949999995	0.8333299760000017	0.0000000000000000
0.4157754023687584	0.3336001253904580	0.1305458400828823
0.4170289346266667	0.8348125326340426	0.2606456801904435
0.2500000000000000	0.1528899970000026	0.0795100030000029
0.2500139605761846	0.6544024010412832	0.2164692693823984
0.2487469765258700	0.1479471923905177	0.3473782392526353
0.2496799979999977	0.4998799860000034	0.0940499980000027
0.2489106271364817	0.9997623835822635	0.2236104071311592
0.2511048962477079	0.5004377804302078	0.3588841826348019
0.2500000000000000	0.8471000190000026	0.0795100030000029
0.2498800207831502	0.3472431869495434	0.2176601853923449
0.2478917050076814	0.8516270449353003	0.3475776382731736

0.0833299980000035	0.5137699839999996	0.0094599999999971
0.0837259120858494	0.0132445273863971	0.1389169579589745
0.0836164868173799	0.5184242151579764	0.2769809659515942
0.0833299980000035	0.8195599909999984	0.0094599999999971
0.0831976526019880	0.3213325475973840	0.1393057936335717
0.0820350576205342	0.8195149777854654	0.2753921579686345
0.0833299980000035	0.1666699949999995	0.0000000000000000
0.0832165328482760	0.6663585693301785	0.1308848681773886
0.0811781409240654	0.1666754926721827	0.2595993647839441

Optimized methane structure coordinates:

a = 15.00000 Å α = 90.0000°

b = 15.00000 Å β = 90.0000°

c = 15.00000 Å γ = 90.0000°

C H

1 4

0.4080378110853579	0.4384116974283478	0.4343628899354117
0.4079485071343817	0.5115675472593658	0.4343592430508548
0.4746173315228771	0.4140481742531243	0.4522205375445904
0.3592043137003089	0.4140659828804318	0.4831127688077719
0.3901120387570731	0.4140666085120550	0.3677545618613718

References

[1] Haas, P.; Tran, F.; Blaha, P., Calculation of the Lattice Constant of Solids with Semilocal Functionals. *Physical Review B* 2009, *79*, 085104.

[2] Bredow, T.; Gerson, A. R., Effect of Exchange and Correlation on Bulk Properties of MgO, NiO, and CoO. *Physical Review B* 2000, *61*, 5194.